## Hoffman 10 631358-History

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FILE 'HCAPLUS' ENTERED AT 19:14:05 ON 10 SEP 2005
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L1
                "KUCERA DAVID JOHN"/AU)
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               D IBIB ABS L1
              D IBIB ABS L1 2-16
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L2
               LEIGH"/AU)
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L36
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L37
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         25543 SEA ABB=ON PLU=ON TOLUENESULFON?
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         82176 SEA ABB=ON PLU=ON L41
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L47
         17976 SEA ABB=ON PLU=ON L42(L)REACT?/RL
L49
         37642 SEA ABB=ON PLU=ON L11
L53
         1370 SEA ABB=ON PLU=ON L12
L54
            45 SEA ABB=ON PLU=ON L42 AND L43 AND (L53 OR L54)
L55
            20 SEA. ABB=ON PLU=ON L42 AND L43 AND L47
L56
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L57
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L58
            37 SEA ABB=ON PLU=ON L58 AND PD=<NOVEMBER 5, 2003
L59
               D STAT OUE
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FILE HCAPLUS

D IBIB ABS HITSTR L59 1-37

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### Hoffman 10 631358-History

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FILE COVERS 1907 - 10 Sep 2005 VOL 143 ISS 12 FILE LAST UPDATED: 8 Sep 2005 (20050908/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

#### FILE REGISTRY

=>

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 8 SEP 2005 HIGHEST RN 862771-58-2 DICTIONARY FILE UPDATES: 8 SEP 2005 HIGHEST RN 862771-58-2

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2005

Please note that search-term pricing does apply when conducting SmartSELECT searches.

\*\*\*\*\*\*\*\*\*

\*

\* The CA roles and document type information have been removed from \*

\* the IDE default display format and the ED field has been added, \*

\* effective March 20, 2005. A new display format, IDERL, is now \*

\* available and contains the CA role and document type information. \*

\*

Structure search iteration limits have been increased. See HELP SLIMITS for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

Page 2

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=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 19:14:05 ON 10 SEP 2005

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PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

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FILE COVERS 1907 - 10 Sep 2005 VOL 143 ISS 12 FILE LAST UPDATED: 8 Sep 2005 (20050908/ED)

New CAS Information Use Policies, enter HELP USAGETERMS for details.

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d stat que l1

L1 16 SEA FILE=HCAPLUS ABB=ON PLU=ON "KUCERA D"/AU OR ("KUCERA DAVID JOHN"/AU)

=> d ibib abs l1

L1 ANSWER 1 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:523413 HCAPLUS

DOCUMENT NUMBER: 143:59813

TITLE: Methods of preparing N-acylpyrrolidinecarboxamides

useful as HIV protease inhibitors

INVENTOR(S): Kucera, David John; Saeed, Nabil Lauze;

Scott, Robert William

PATENT ASSIGNEE(S): Pfizer Inc., USA

SOURCE: PCT Int. Appl., 108 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.				KIND DATE				APPLICATION NO.							DATE			
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WO 2005	0541	87		A1		2005	0616	1	WO 2	004-	IB38	10		2	0041	122		
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	CN,	CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	EG,	ES,	FI,	GB,	GD,		
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	NO,	NZ,	OM,	PG,	PH,	PL,	PT,	RO,	RU,	SC,	SD,	SE,	SG,	SK,	SL,	SY,		
	ТJ,	TM,	TN,	TR,	TT,	TZ,	UA,	ŪĠ,	US,	UZ,	VC,	VN,	ΥU,	ZA,	ZM,	zw		
RW:	BW,	GH,	GM,	ΚE,	LS,	MW,	MZ,	NA,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	AM,		
	AZ,	BY,	KG,	KZ,	MD,	RU,	ТJ,	TM,	AT,	BE,	BG,	CH,	CY,	CZ,	DE,	DK,		
	EE,	ES,	FI,	FR,	GB,	GR,	HU,	ΙE,	IS,	IT,	LU,	MC,	NL,	PL,	PT,	RO,		
	SE,	SI,	SK,	TR,	BF,	ВJ,	CF,	CG,	CI,	CM,	GΑ,	GN,	GQ,	GW,	ML,	MR,		

NE, SN, TD, TG

US 2005153903 A1 20050714 US 2004-3948 20041203 PRIORITY APPLN. INFO.: US 2003-527470P P 20031204 US 2004-591354P P 20040726

OTHER SOURCE(S): MARPAT 143:59813

GΙ

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The invention relates to methods of preparing compds. of formula I that are useful (no data) as inhibitors of the HIV protease enzyme. In compds. I, R1 is Ph optionally substituted by at least one substituent independently selected from C1-6 alkyl, OH, C1-6 alkylcarbonyloxy, C6-10 arylcarbonyloxy, and heteroarylcarbonyloxy; R2 is C2-6 alkenyl or C1-6 alkyl optionally substituted with at least one halogen; R3 is a hydroxyl protecting group; R4, R5, R6, and R7 are independently selected from H and C1-6 alkyl; and R8 is H or C1-4 alkyl. (2S,3S)-3-Amino-2-hydroxy-4-phenylbutyric acid was coupled with 3-acetoxy-2-methylbenzoyl chloride followed by acetylation and crystallization to give pure II. II underwent coupling with the hydrochloride of III (preparation given) using thionyl chloride, followed by hydrolysis of acetates and crystallization to give IV.

The

one-pot preparation of II is also demonstrated on a large scale (110 kg, 563 mol of aminohydroxyphenylbutyric acid). X-ray diffraction and Raman scattering spectra of the target compds. were collected and are included as figures. Previous methods for preparing these types of compds. were linear, whereas the invention provides convergent synthetic routes with maximized efficiency.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d ibib abs 11 2-16

L1 ANSWER 2 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:497500 HCAPLUS

DOCUMENT NUMBER: 143:43873

TITLE: Methods of preparing (4R)-3-[(2S,3S)-2-hydroxy-3-(3-

hydroxy-2-methylbenzoylamino)-4-phenylbutyryl]-5,5-dimethylthiazolidine-4-carboxamides useful as HIV

protease inhibitors

INVENTOR(S): Kucera, David John; Scott, Robert William

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA

SOURCE: U.S. Pat. Appl. Publ., 39 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND DAT	ATE APPL	ICATION NO.	DATE						
US 2005124673	A1 200	050609 US 20	US 2004~3952							
WO 2005054214	A1 200	050616 WO 20	004-IB3823	20041122						
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CN, CO, CR,	CU, CZ, DE	DE, DK, DM, DZ,	EC, EE, EG, ES,	FI, GB, GD,						
GE, GH, GM,	HR, HU, II	D, IL, IN, IS,	JP, KE, KG, KP,	KR, KZ, LC,						

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US 2003-527477P

P 20031204

PRIORITY APPLN. INFO.:
OTHER SOURCE(S): MARPAT 143:43873

GT

\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

The invention relates to methods of preparing compds. of formula (I) [R1 = Ph AB optionally substituted by at least one substituent independently chosen from C1-6 alkyl, HO, C1-6 alkylcarbonyloxy, C6-10 arylcarbonyloxy, and heteroarylcarbonyloxy; R2 = C2-6 alkenyl, C1-6 alkyl optionally substituted with at least one halogen, or -(CR4R5)nR8; n = an integer from 0 to 5; R2' = H or C1-4 alkyl; Z = S, 0, S0, S02, CH2, or CFH; R3 = H or a hydroxy protecting group; each R4, R5, R6, and R7 are independently selected from H and C1-6 alkyl; R8 = C6-10 aryl optionally substituted at least one substituent selected from C1-6 alkyl, hydroxy, and halogen] which comprises reacting a compound of formula (II) (wherein Y1 = HO or a leaving group; R1 and R3 are as described above) with a compound of formula (III) (R2, R2', Z, and R4-R7 are as described above) or salts or solvates thereof. These compds. are useful as inhibitors of the HIV protease enzyme (no data). The present invention also relates to intermediate compds. useful in the preparation of compds. of formula I. Thus, 271 g (2S, 3S) -3-(3-acetoxy-2-methylbenzoylamino) -2-hydroxy-4-phenylbutyric acid, 161 g (4R)-5,5-dimethylthiazolidine-4-carboxylic acid N-(allyl)amide, and 32.6 g HOBt.H2O were dissolved in 2-methyltetrahydrofuran 1,750 mL, treated portionwise with 119 mL diisopropylcarbodiimide at 30 min intervals and then with 100 g celite, and stirred at room temperature for 3 h to

give , after workup, a 1.35 L solution of acetic acid 3-[[(1S,2S)-3-((4R)-4-allylcarbamoyl-5,5-dimethylthiazolidin-3-yl)-1-benzyl-2-hydroxy-3-oxopropyl]carbamoyl]-2-methylphenyl ester (IV) (R = Ac)in 2-methyltetrahydrofuran. MeOH (330 L) and 66.9 g K2CO3 were sequentially added to the solution of IV (R = Ac) (405 g) and the resulting mixture was stirred at room temperature for 2.5 h, treated with addnl. 20 g K2CO3, and stirred for 3 h to give, after workup, 204 g (4R)-3-[(2S,3S)-2-hydroxy-3-(3-hydroxy-2-methylbenzoylamino)-4-phenylbutyryl]-5,5-dimethylthiazolidine-4-carboxylic acid N-(allyl)amide IV (R = H).

L1 ANSWER 3 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:99173 HCAPLUS

DOCUMENT NUMBER: 142:197575

TITLE: Process for preparation of chiral 1,2-diaminopropanes

and thiazole compounds containing them.

Kucera, David John; Yvon, Brigitte Leigh

INVENTOR(S): Kucera, David John; Yvon, Brigitte PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA SOURCE: U.S. Pat. Appl. Publ., 20 pp.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE: Facence English

FAMILY ACC. NUM. COUNT: 1

### PATENT INFORMATION:

DATE APPLICATION NO. DATE PATENT NO. KIND \_\_\_\_\_ \_\_\_\_\_ \_ \_ \_ \_ -----------20050203 US 2003-631358 US 2005026966 A1 20030730 PRIORITY APPLN. INFO.: US 2003-631358 20030730 CASREACT 142:197575; MARPAT 142:197575 OTHER SOURCE(S): GI

$$R^3R^2N$$
 $NH_2$  .2TSOH I
 $NH_2$   $NH$ 

Title compds. [I; R1-R3 = H, (substituted) alkyl, heteroalkyl, AB (CR13R14)tX; t = 1-5; X = aryl, cycloalkyl, heterocyclyl; R13, R14 = H, alkyl, heteroalkyl], were prepared by treatment of amino acid derivs. (II) with R2R3NH (R1-R3 as above) to give the corresponding amides followed by N-deprotection, reduction, and conversion to the tosylate salts. I are intermediates in preparation of thiazole derivs. (III; R1-R3 as above; R4, R5 = H, halo, alkyl, OMe, OH, NH2, NHMe, NMe2, NO2, SH, SMe, SOMe, SO2Me, PMe2, PO3H2; R6, R7 = H, halo, MeO, alkyl; X = C, N). Thus, Z-D-Ala-OH and HOBt.H2O in MeCN at -3° were treated with DCC in MeCN and then with Me2NH.HCl and diisopropylethylamine followed by stirring at 0° for 1.5 h, warming to room temperature, and stirring overnight to give 79% N-benzyloxycarbonyl-D-alanine dimethylamide. The latter was hydrogenolyzed in EtOH over Pd/C at 45 psi H2 to give 83% D-alanine dimethylamide. This was refluxed 17 h with LiAlH4 in THF followed by salification with p-TsOH to give 69.5% (R)-1-dimethylaminoprop-2-ylamine. bistosylate.

L1 ANSWER 4 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

PATENT ASSIGNEE(S):

2004:857219 HCAPLUS

DOCUMENT NUMBER:

141:314632

TITLE:

Preparation of amino acid amides as HIV protease

inhibitors

INVENTOR(S):

Kucera, David John; Scott, Robert William

Agouron Pharmaceuticals, Inc., USA

SOURCE:

U.S. Pat. Appl. Publ., 296 pp., Cont.-in-part of U.S.

Ser. No. 166,979.

CODEN: USXXCO

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

### PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE		
US 2004204591	A1	20041014	US 2003-729645	20031204		
US 2003225071	A1	20031204	US 2002-166979	20020611		
ZA 2003009041	Α	20040722	ZA 2003-9041	20031120		
PRIORITY APPLN. INFO.:			US 2001-297460P P	20010611		
			US 2001-297729P P	20010611		
			US 2002-166979 A2	20020611		

OTHER SOURCE(S):

MARPAT 141:314632

GI

AB Synthetic amides I [R1 is a 5- or 6-membered monocyclic carbo- or heterocyclic ring which is optionally substituted by alkyl, hydroxyl, alkylcarbonyloxy, arylcarbonyloxy or heteroarylcarbonyloxy; R2 is haloalkyl; R4-R7 are H or alkyl] or their pharmaceutically-active salts, metabolites or prodrugs are useful as inhibitors of the HIV protease enzyme. Thus, pyrrolidinecarboxamide derivative II was prepared via amidation reactions. A combinatorial chemical approach to HIV protease inhibitors was also presented.

II

L1 ANSWER 5 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:722954 HCAPLUS

DOCUMENT NUMBER:

141:243832

TITLE:

Preparation of amino acid amides as HIV protease

inhibitors

INVENTOR(S):

Kucera, David John; Scott, Robert William

PATENT ASSIGNEE(S): Pfizer Inc, USA

SOURCE:

U.S. Pat. Appl. Publ., 120 pp., Cont.-in-part of U.S.

Ser. No. 166,957.

CODEN: USXXCO

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 2004171842	A1	20040902	US 2003-728602	20031204
US 2003153507	A1	20030814	US 2002-166957	20020611
ZA 2003009041	Α	20040722	ZA 2003-9041	20031120
PRIORITY APPLN. INFO.:			US 2001-297460P P	20010611
			US 2001-297729P P	20010611
			US 2002-166957 A2	20020611

OTHER SOURCE(S): CASREACT 141:243832; MARPAT 141:243832

GI

AB Synthetic amides I [R1 is (un) substituted carbo- or heterocyclic; R2 is (un) substituted alkyl, alkenyl, alkynyl, Ph, phenylalkyl, phenylalkenyl, or phenylalkynyl; R2', R3-R7 are H or (un) substituted alkyl; X is (un) substituted Ph; Z is S, O, SO, SO2, CH2, or CHF; R8, R8' are H, halo, an aliphatic or haloaliph. group (with provisos)] inhibit or block the biol. activity of the HIV protease. Thus, thiazolidinecarboxamide derivative II was prepared via amidation reactions and showed Ki = 1.7 nM for inhibition of HIV-1 protease. A combinatorial chemical approach to HIV protease inhibitors was also presented.

L1 ANSWER 6 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:891973 HCAPLUS

DOCUMENT NUMBER: 139:365102

TITLE: Methods for the preparation of taxanes using

 $\beta$ -lactam intermediates

INVENTOR(S): Thottathil, John K.; Trifunovich, Ivan D.;

Kucera, David J.; Li, Wen-Sen

PATENT ASSIGNEE(S): Bristol-Myers Squibb Company, USA

SOURCE: Eur. Pat. Appl., 29 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

	KIND		APPLICATION NO.	DATE				
EP 1361222	A1	20031112	EP 2003-8433 GB, GR, IT, LI, LU,					
			IL 1994-123063					
EP 617018	A1	19940928	EP 1994-301809					
EP 617018	B1	20031001						
R: AT, BE,	CH, DE,	DK, ES, FR,	GB, GR, IE, IT, LI,	LU, MC, NL, PT, SE				
HU 72646			HU 1995-2449	19940318				
US 6350886	B1	20020226	US 1995-439920	19950512				
US 6350887	B1	20020226	US 1995-440291	19950512				
US 6310201			US 1999-330452	19990611				
US 2002137927	A1	20020926	US 2001-6599	20011205				
US 2005107605	A1	20050519	US 2004-969693	20041020				
PRIORITY APPLN. INFO.	:		US 1993-33598	A 19930319				
			EP 1994-301809	A3 19940314				
			IL 1994-108763	A3 19940224				
			HU 1994-803	A 19940318				
			US 1994-320628	B3 19941011				
			US 1995-440291	A1 19950512				
			US 1997-878234	B1 19970618				
			US 2001-6599	B1 20011205				

OTHER SOURCE(S): MARPAT 139:365102

GΙ

AB Novel side-chain-bearing taxane derivs., such as I [R1, R2 = alkyl; CaR1R2= cycloalkyl, cycloalkenyl, heterocycle; wherein the carbon atom marked as Ca to which R1 and R2 are bonded is non-asym.; R3 = alkyl; R4 = aryl; R5 = H, arylcarbonyl, alkoxycarbonyl; R7 = H, alkylcarbonyl, hydroxyl protecting group; R8 = H, hydroxyl protecting group], were prepared using  $\beta$ -lactam intermediates as side chain precursors. The present invention also relates to novel methods of coupling the  $\beta$ -lactam intermediates to form the aforementioned taxanes, and to methods of preparing the  $\beta$ -lactams. Thus, taxol was prepared via a multistep reaction sequence starting from (3R-cis)-3-acetyloxy-4-phenyl-2-azetidinone and

Ι

10-desacetylbaccatin III.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 7 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:964341 HCAPLUS

DOCUMENT NUMBER: 138:39545

TITLE: Preparation of amino acid amides as HIV protease

inhibitors

INVENTOR(S): Canon-Koch, Stacie S.; Alexander, Therese N.; Barvian,

Mark; Bolton, Gary; Boyer, Fredrick E.; Burke,

Benjamin J.; Holler, Tod; Jewell, Tanya M.; Prasad,

Josyula Vara; Kucera, David J.; Machak,

Jeff; Mitchell, Lennert J.; Murphy, Sean T.; Reich, Siegfried H.; Skalitzky, Donald J.; Tatlock, John H.; Varney, Michael D.; Virgil, Scott C.; Worland, Stephen

T.; Melnick, Michael; Linton, Maria A.; Webber,

Stephen E.

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 165 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

PA	PATENT NO.					KIND DATE			APPLICATION NO.						DATE			
_			-					WO 2002-US18548						20020611				
WO																		
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OTHER SOURCE(S): MARPAT 138:39545

GI

AB Synthetic amides I [R1 is an (un)substituted carbo- or heterocyclic group; R2 is (un)substituted alkyl, alkenyl, alkynyl, Ph, phenylalkyl, phenylalkenyl, or phenylalkynyl; R2', R3-R7 are H or (un)substituted alkyl; X is (un)substituted Ph; Z is S, O, SO, SO2, CH2, or CHF; R8, R8' are H, halo, an aliphatic or haloaliph. group (with provisos)] inhibit or block the biol. activity of the HIV protease. Thus, thiazolidinecarboxamide derivative II was prepared via amidation reactions and showed Ki = 1.7 nM for inhibition of HIV-1 protease. A combinatorial chemical approach to HIV protease inhibitors was also presented.

REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L1 ANSWER 8 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:964340 HCAPLUS

DOCUMENT NUMBER: 138:39544

TITLE: Preparation of amino acid amides as HIV protease

inhibitors

INVENTOR(S): Canon-Koch, Stacie S.; Alexander, Therese N.; Barvian,

Mark; Bolton, Gary; Boyer, Fredrick E.; Burke, Benjamin J.; Holler, Tod; Jewell, Tanya M.; Prasad,

Josyula Vara; Kucera, David J.; Linton,

Maria A.; Machak, Jeff; Mitchell, Lennert J.; Murphy, Sean T.; Reich, Siegfried H.; Skalitzky, Donald J.; Tatlock, John H.; Varney, Michael D.; Virgil, Scott C.; Webber, Stephen E.; Worland, Stephen T.; Melnick,

Michael

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 306 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 4

PATENT INFORMATION:

		APPLICATION NO.	DATE			
WO 2002100844 WO 2002100844	A2 20021219	WO 2002-US18717	20020611			
CO, CR, CU, GM, HR, HU, LS, LT, LU, PL, PT, RO, UA, UG, UZ, RW: GH, GM, KE, CY, DE, DK,	CZ, DE, DK, DM, ID, IL, IN, IS, LV, MA, MD, MG, RU, SD, SE, SG, VN, YU, ZA, ZM, LS, MW, MZ, SD, ES, FI, FR, GB,	BA, BB, BG, BR, BY, DZ, EC, EE, ES, FI, JP, KE, KG, KP, KR, MK, MN, MW, MX, MZ, SI, SK, SL, TJ, TM, ZW, AM, AZ, BY, KG, SL, SZ, TZ, UG, ZM, GR, IE, IT, LU, MC,	GB, GD, GE, GH, KZ, LC, LK, LR, NO, NZ, OM, PH, TN, TR, TT, TZ, KZ, MD, RU, TJ, TM ZW, AT, BE, CH, NL, PT, SE, TR,			
		GN, GQ, GW, ML, MR, EP 2002-746518				
	DE, DK, ES, FR, LV, FI, RO, MK,	GB, GR, IT, LI, LU, CY, AL, TR	NL, SE, MC, PT,			
BR 2002010358	A 20040622	BR 2002-10358				
		JP 2003-503612				
PRIORITY APPLN. INFO.:	A 20040722	ZA 2003-9041 US 2001-297460P				
INIONIII IIII BINI III ON		US 2001-297729P				
		WO 2002-US18717	W 20020611			
OTHER SOURCE(S):	MARPAT 138:3954	4				

GI

AB Synthetic amides I [R1 is an aliphatic, carbo- or heterocyclic group, OR1', SR1', NHR1', NR1'R1'', or COR1', where R1' is an aliphatic, carbo- or heterocyclic group and R1'' is H or an aliphatic group or NR1'R1" is (un) substituted heterocyclyl; V is CO, CS, or SO2; R2 is an aliphatic,

carbocyclic, or carbocyclic aliphatic group, or NR2aR2b, where R2a is an aliphatic, carbo-, or heterocyclic group and R2b is H or an aliphatic group; W is N, O, C, or CH; R2' is H or an aliphatic group (when W is N, C or CH) or R2R2'W is an (un) substituted carbo- or heterocyclic ring; R2 is absent when W is O; X is (un)substituted Ph, phenoxy, phenylthio, benzyl, or phenethyl; R8, R8' are H, halo, or an aliphatic group; A is CH2, CHRA, or is absent; Z is S, O, SO2, CH2, CHF, CF2, CHOH, CH(ORZ), CH(NRZRZ'), CH(SRZ), CO, or CHRZ, where RZ is an aliphatic, carbo-, or heterocyclic group and RZ' is H or an aliphatic group; or RA and RZ taken together with A and Z form an (un) substituted carbo- or heterocyclic ring; R3 is H or an aliphatic group; R4, R5 are H, halo, an aliphatic or acyl group group; R4 may combine with R5 or with R6 or R7 to form a ring; R6, R7 are H or an aliphatic group] inhibit or block the biol. activity of the HIV protease. Thus, thiazolidinecarboxamide derivative II was prepared via amidation reactions and showed Ki = 0.21 nM for inhibition of HIV-1 protease. A combinatorial chemical approach to HIV protease inhibitors was also presented.

L1 ANSWER 9 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:382780 HCAPLUS

DOCUMENT NUMBER: 125:58741

TITLE: Preparation of phosphonosulfonate salts as squalene

synthetase inhibitors

INVENTOR(S): Pendri, Yadagiri; Chen, Chung-Pin; Kucera, David

J.; Martinez, Eduardo J.; Pansegrau, Paul D.;

Thottathil, John K.; Timmins, Peter Bristol-Myers Squibb Company, USA

PATENT ASSIGNEE(S): Bristol-Myers Squibb Co SOURCE: Eur. Pat. Appl., 13 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent

LANGUAGE: Factive English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

P	ATENT NO.		KIND	DATE	APPLICATION NO.	DATE
_						
E	P 710665		A1	19960508	EP 1995-307618	19951026
	R: AT,	BE, CH,	DE, DK	, ES, FR,	GB, GR, IE, IT, LI,	LU, MC, NL, PT, SE
С	A 2159850		AA	19960504	CA 1995-2159850	19951004
J	P 08208672		A2	19960813	JP 1995-280397	19951027
F	I 9505256		A	19960504	FI 1995-5256	19951102
N	0 9504389		A	19960506	NO 1995-4389	19951102
A	U 9534587		A1	19960509	AU 1995-34587	19951102
H	U 73140		A2	19960628	HU 1995-3136	19951102
C	N 1130188		A	19960904	CN 1995-119023	19951103
Z	A 9509326		A	19970505	ZA 1995-9326	19951103
PRIORI	TY APPLN.	INFO.:			US 1994-333661	A 19941103
GT						

Ι

AB New salt forms of the phosphonosulfonate squalene synthetase inhibitor I are provided wherein X represents Ca, t-butylamine salt, t-octylamine salt and dehydrodroabietylamine salt. These salts inhibit cholesterol biosynthesis and therefore were proposed in lowering serum cholesterol and in treating atherosclerosis (no data).

L1 ANSWER 10 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:315691 HCAPLUS

DOCUMENT NUMBER: 122:106194

TITLE: Beta-lactams, methods for the preparation of taxanes,

and sidechain-bearing taxanes

INVENTOR(S): Thottathil, John K.; Trifunovich, Ivan D.;

DATE

Kucera, David J.; Li, Wen-Sen
Bristol-Myers Squibb Co., USA

APPLICATION NO

DATE

SOURCE: Eur. Pat. Appl., 27 pp.

KIND

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

DATENT NO

PATENT ASSIGNEE(S):

		TENT NO.			KINI		DATE			PLICATION NO.		D	ATE		
		617018					19940928			1994-301809		1	9940.	314	
	EP	617018			В1		20031001								
		R: AT,	BE,	CH,	DE,	DK	, ES, FR,	GB,	GF	R, IE, IT, LI,	LU,	MC,	NL,	PT,	SE
	TW	467896			В		20011211		TW	1994-83101294		1	9940	217	
	CA	2116093			AA		19940920		CA	1994-83101294 1994-2116093		1	9940	221	
		108763			A1		19980715		IL	1994-108763		1	9940	224	
	$_{ m IL}$	123063			A1		20000217			1994-123063					
	ΑT	251134			E		20031015		ΑТ	1994-301809		1	9940	314	
	ΕP	1361222			A1		20031112		ΕP	2003-8433		1	9940	314	
		R: AT,	BE,	CH,	DE,	DK	EC ED	GB.	GF	R, IT, LI, LU,	NL,	SE,	MC,	PT,	ΙE
	PT	617018			T T3 A A1 B2 A2 A2 A B A2 B1		20040227		PT	1994-301809 1994-301809 1994-1286 1994-57919		1	9940	314	
	ES	2208649			Т3		20040616		ES	1994-301809		1	9940	314	
	FI	9401286			Α		19940920		FΙ	1994-1286		1	9940	318	
	AU	9457919			A1		19940922		ΑU	1994-57919		1	9940	318	
	AU	676879			В2		19970327								
	HU	69733			A2		19950928		HU	1994-803		1	9940	318	
	HU	72646			A2		19960528		HU	1994-803 1995-2449		1	9940	318	
	CN	1097416			Α		19950118		CN	1994-102895		1	9940	319	
	CN	1080256			В		20020306								
	JP	06321896			A2		19941122		JР	1994-50253		1	9940	322	
	US	6350886			B1		20020226		US	1995-439920		1	9950	512	
	US	6350887			B1		20020226		US	1995-440291					
	HK	1002005			A1		20040305		ΗK	1998-100740		1	9980	127	
	US	6310201			B1		20011030		US	1999-330452		1	9990	611	
	CN	1271729			Α		20001101			2000-104016					
	US	200213792	27		A1		20020926		US	2001-6599		2	0011	205	
	US	200510760	)5		A1		20050519		US	2004-969693		2	0041	020	
PRIO	RIT	Y APPLN.	INFO	. :					US	1993-33598	1	1	9930	319	
									IL	1994-108763	1	A3 1	9940	224	
									EΡ	1994-301809	1	A3 1	9940	314	
									HU	1994-803	1	<b>A</b> 1	9940	318	
									US	1994-320628	I	33 1	9941	011	
									US	1995-440291	1	A1 1	9950	512	
									US	1997-878234	I	31 1	9970	618	
									US	2001-6599	I	31 2	0011	205	

OTHER SOURCE(S):

CASREACT 122:106194; MARPAT 122:106194

GI

AB β-Lactams I [R1 = R2 = same alkyl; or R1R2 = atoms to form cycloalk(en)yl or heterocyclo group; R3 = alkyl; R4 = aryl; R5 = H, arylcarbonyl, alkoxycarbonyl] are useful as intermediates in the preparation of sidechain-bearing taxanes such as taxol and taxotere. The invention also relates to novel methods of coupling the β-lactams, and to certain novel sidechain-bearing taxanes which result. For example, (3R-cis)-3-hydroxy-4-phenyl-2-azetidinone underwent protection of hydroxy with 2-methoxypropene or Me2C(OMe)2 (up to 90% yield) and N-benzoylation with BzCl (73.7%) to give title lactam II. Then, 7-O- (triethylsilyl)baccatin III [preparation given] in THF was cooled to -50°, deprotonated with LiN(SiMe3)2, and treated with II in THF, to give crystalline taxol derivative III [R6 = CMe2OMe, R7 = SiEt3] containing some

partially deprotected material (R6 = H) in 89-95% yield. Final deprotection with either dilute aqueous HCl in cold EtOH-THF, or with 48% aqueous HF

in MeCN-pyridine, gave III [R6 = R7 = H], i.e. taxol, in roughly 92-100% yield.

L1 ANSWER 11 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:408747 HCAPLUS

DOCUMENT NUMBER: 121:8747

TITLE: Synthesis of oxepanes by Prins cyclizations. Formation

of spirocyclic or bridged ring systems by

intramolecular Heck reactions

AUTHOR(S): Kucera, David John

CORPORATE SOURCE: Univ. California, Irvine, CA, USA

SOURCE: (1991) 322 pp. Avail.: Univ. Microfilms Int., Order

No. DA9217262

From: Diss. Abstr. Int. B 1992, 53(1), 283

DOCUMENT TYPE: Dissertation LANGUAGE: English

AB Unavailable

L1 ANSWER 12 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:107386 HCAPLUS

DOCUMENT NUMBER: 120:107386

TITLE: Total synthesis of (±)-scopadulcic acid A. An

illustration of the utility of palladium catalyzed

polyene cyclizations

AUTHOR(S): Kucera, David J.; O'Connor, Stephen J.;

Overman, Larry E.

CORPORATE SOURCE: Dep. Chem., Univ. California, Irvine, CA, 92717-2025,

USA

SOURCE: Journal of Organic Chemistry (1993), 58(20), 5304-6

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 120:107386

GI

#### \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB The first total synthesis of (±)-scopadulcic acid A (I) is described. A divinylcyclopropane rearrangement is the key step in assembling the methylenecycloheptene cyclization substrate II. The key palladium catalyzed polyene cyclization of II was accomplished on a multi-gram scale, with complete stereochem. fidelity, to provide the tricyclic intermediate III in 31% overall yield from the mixture of cyclopropyl bromides IV. The A-ring is formed by intramol. aldol cyclization of V to give enone VI. This tetracyclic enone is a potentially versatile intermediate for the synthesis of a wide variety of scopadulan diterpenes and analogs. The more efficient second generation total synthesis entry to the scopadulan diterpenes reported here will facilitate systematic studies of the mol. basis for the diverse biol. activity observed in this series as well as illustrate further the power of palladium-catalyzed polyene cyclizations in the construction of complex mols.

L1 ANSWER 13 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:168404 HCAPLUS

DOCUMENT NUMBER: 118:168404

TITLE: Palladium-catalyzed polyene cyclizations

AUTHOR(S): Overman, Larry E.; Abelman, Matthew M.; Kucera,

David J.; Tran, Vinh D.; Ricca, Daniel J.

CORPORATE SOURCE: Dep. Chem., Univ. California, Irvine, CA, 92717, USA SOURCE: Pure and Applied Chemistry (1992), 64(12), 1813-19

CODEN: PACHAS; ISSN: 0033-4545

DOCUMENT TYPE: Journal; General Review

LANGUAGE: English

AB A review with 23 refs. Palladium-catalyzed cyclizations of polyene aryl halides or enol triflates provide ready access to a wide variety of polycyclic carbon skeletons. General features of this chemical as well as stereochem. aspects are discussed. The power of this organometallic chemical is illustrated by the facile construction of the tetracyclic ring system

of the scopadulcic acids.

L1 ANSWER 14 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:11906 HCAPLUS

DOCUMENT NUMBER: 118:11906

TITLE: Acoustic impedance measurements of transverse and

longitudinal sound in superfluid helium-3

AUTHOR(S): Kalbfeld, S.; Kucera, D.; Ketterson, J. B.

CORPORATE SOURCE: Dep. Phys. Astron., Northwestern Univ., Evanston, IL,

60208, USA

SOURCE: Journal of Low Temperature Physics (1992), 89(3-4),

735-8

CODEN: JLTPAC; ISSN: 0022-2291

DOCUMENT TYPE: Journal LANGUAGE: English

AB Simultaneous acoustic impedance measurements are presented of transverse and longitudinal sound at 61 MHz and pressures of 15.6, 10.5, and 8.0 bar.

L1 ANSWER 15 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:632547 HCAPLUS

DOCUMENT NUMBER: 111:232547

TITLE: Preparation of seven-membered ring cyclic ethers and

3-alkylidenetetrahydropyrans from the cyclization of

oxonium cations derived from unsubstituted and

silicon-containing 4-alken-1-ols

AUTHOR(S): Castaneda, Armando; Kucera, David J.;

Overman, Larry E.

CORPORATE SOURCE: Dep. Chem., Univ. California, Irvine, CA, 92717, USA

SOURCE: Journal of Organic Chemistry (1989), 54(24), 5695-707

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE: Journal

LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:232547

GI

Lewis acid promoted cyclization of mixed acetals derived from 4-alken-1-ols provides direct access to seven- or six-membered cyclic ethers. Ring size is determined primarily by the electronic bias of the alkene participant. Of particular significance are the formation of 2,3,6,7-tetrahydrooxepins I (R = H, HCH2CH2) from the cyclization of acetals H2C:C(SiMe3)CH2CH2CHROR1 [II; R = H, PhCH2CH2, R1 = CH(OMe)CH2CH2Ph; R = PhCH2CH2, R1 = CH2CH2OMe], the completely stereoselective formation of the cis-2,7-disubstituted-2,3,6,7-tetrahydrooxepin I (R = PhCH2CH2) from II [R = PhCH2CH2, R1 = CH(OMe)CH2CH2Ph], and the stereospecific cyclization of acetals derived from (E)- or (Z)-4-nonen-1-ol to afford the (E)- or (Z)-pentylidenetetrahydropyrans (E)-III and (Z)-III, resp. The divergent behavior of acetals (Z)-MeSiCH:CHCH2CH2CH(OR2)CH2CH2Ph (R2 = CH2OCH2CH2OMe, CHMeOMe) and more complex rearrangement pathways.

L1 ANSWER 16 OF 16 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:632155 HCAPLUS

DOCUMENT NUMBER: 111:232155

TITLE: Palladium-catalyzed polyene cyclizations of trienyl

triflates

AUTHOR(S): Carpenter, Nancy E.; Kucera, David J.;

Overman, Larry E.

CORPORATE SOURCE: Dep. Chem., Univ. California, Irvine, CA, 92717, USA

SOURCE: Journal of Organic Chemistry (1989), 54(25), 5846-8

CODEN: JOCEAH; ISSN: 0022-3263

I

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 111:232155

GI

$$CH_2CH_2C (=CH_2) CH_2 (CH_2) nCH = CH_2$$

CH<sub>2</sub>) n

II

AB (Methylenealkenyl)cyclohexanedione enol triflates I (n = 1, 2) were treated with Pd(OAc)2-Ph3P in MeCN containing Et3N to give spirocycloalkaneindans II.

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L1 16 SEA FILE=HCAPLUS ABB=ON PLU=ON "KUCERA D"/AU OR ("KUCERA

DAVID J"/AU OR "KUCERA DAVID JOHN"/AU)

L2 5 SEA FILE=HCAPLUS ABB=ON PLU=ON ("YVON BRIGITTE L"/AU OR

"YVON BRIGITTE LEIGH"/AU)

L3 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L2 NOT L1

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L3 ANSWER 1 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:337764 HCAPLUS

DOCUMENT NUMBER: 143:26151

TITLE: The complex photochemistry of 2,3-

dibenzylidenesuccinates

AUTHOR(S): Assoumatine, Tokoure; Yvon, Brigitte L.;

Charlton, James L.

CORPORATE SOURCE: Department of Chemistry, University of Manitoba,

Winnipeg, MB, R3T 2N2, Can.

SOURCE: Canadian Journal of Chemistry (2004), 82(12),

1663-1667

CODEN: CJCHAG; ISSN: 0008-4042

PUBLISHER: National Research Council of Canada

DOCUMENT TYPE: Journal LANGUAGE: English

AB The photochem. of di-Et E,E-2,3-(3,4,5-trimethoxybenzylidene) succinate (8) is solvent dependent. In both protic and aprotic solvents, there is a photoequil. established between 8 and its E,Z-isomer (9). In chloroform at high light intensity, very little 9 is formed and the main product is 1,4-dihydronaphthalene (10), formed via photoinduced intramol. [1,3]-sigmatropic hydrogen shift within an intermediate

1,8a-dihydronaphthalene (11). In protic solvents, irradiation of either 8 or 9 ultimately gives primarily the cis-1,2-dihydronaphthalene product (13), along with smaller amts. of the trans isomer (14). By using deuterated solvents, 13 and 14 are formed by solvent protonation (or deuteration) of the 1,8a-dihydronaphthalene intermediate (11 or 12).

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 2 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:406651 HCAPLUS

DOCUMENT NUMBER: 141:123492

TITLE: A Short Asymmetric Synthesis of (+)-Lyoniresinol

Dimethyl Ether

AUTHOR(S): Assoumatine, Tokoure; Datta, Probal K.; Hooper,

Timothy S.; Yvon, Brigitte L.; Charlton,

James L.

CORPORATE SOURCE: Department of Chemistry, University of Manitoba,

Winnipeg, MB, R3T 2N2, Can.

SOURCE: Journal of Organic Chemistry (2004), 69(12), 4140-4144

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

Ι

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 141:123492

GI

AB A short, efficient synthesis of the lignan (+)-lyoniresinol di-Me ether (I) is described. The synthesis is achieved by asym. photocyclization of an achiral dibenzylidenesuccinate to a chiral aryldihydronaphthalene. (-)-Ephedrine is used as a chiral auxiliary to bias the atropisomeric equilibrium in the dibenzylidenesuccinate prior to the photochem. reaction. The synthesis of the title compound was accomplished in five steps, and the final product was recrystd. to constant m.p. and rotation.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS

#### RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:823650 HCAPLUS

DOCUMENT NUMBER: 136:102224

TITLE: Acid-catalyzed cyclization of 2,3-

dibenzylidenesuccinates: synthesis of lignans

(±)-cagayanin and (±)-galbulin

AUTHOR(S): Datta, Probal K.; Yau, Chi; Hooper, Timothy S.;

Yvon, Brigitte L.; Charlton, James L.

CORPORATE SOURCE: Department of Chemistry, University of Manitoba,

Winnipeg, MB, R3T 2N2, Can.

SOURCE: Journal of Organic Chemistry (2001), 66(25), 8606-8611

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 136:102224

GT

AB Acid-catalyzed cyclizations of E,E-dibenzylidenesuccinate esters, e.g. I,

have been developed as an efficient synthetic route to

1-aryl-1,2-dihydronaphthalenes, e.g. II. This reaction has been used in the synthesis of the naturally occurring lignans ( $\pm$ )-cagayanin and

(±)-galbulin.

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS

RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L3 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2001:584428 HCAPLUS

DOCUMENT NUMBER: 135:303720

TITLE: Synthesis of magnoshinin and cyclogalgravin: modified

Stobbe condensation reaction

AUTHOR(S): Yvon, Brigitte L.; Datta, Probal K.; Le,

Trung N.; Charlton, James L.

CORPORATE SOURCE: Department of Chemistry, University of Manitoba,

Winnipeg, MB, R3T 2N2, Can.

SOURCE: Synthesis (2001), (10), 1556-1560

CODEN: SYNTBF; ISSN: 0039-7881

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 135:303720

GI

AB The development of new methods for lignan synthesis is reported. A recently reported method for the preparation of 1-aryl-1,2-dihydronaphthalenes is exploited to prepare magnoshinin (I) (R = OMe), a naturally occurring lignan, and cyclogalgravin I (R = H) (II) (3,4-dehydrogalbulin), a derivative

of a natural lignan. REFERENCE COUNT:

THERE ARE 29 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

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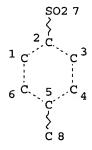
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L2 5 SEA FILE=HCAPLUS ABB=ON PLU=ON ("YVON BRIGITTE L"/AU OR

"YVON BRIGITTE LEIGH"/AU)

29

L3 4 SEA FILE=HCAPLUS ABB=ON PLU=ON L2 NOT L1 L13 STR



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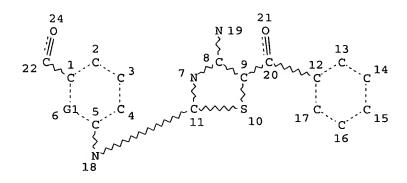
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS 8

STEREO ATTRIBUTES: NONE L15 STR



VAR G1=C/N NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

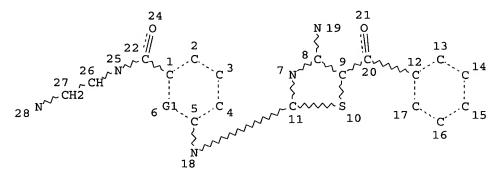
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L18 365356 SEA FILE=REGISTRY SSS FUL L13 OR L15

L25 STR



VAR G1=C/N NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 27

STEREO ATTRIBUTES: NONE

L26 1 SEA FILE=REGISTRY SUB=L18 SSS FUL L25 L30 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L26

L35 1 SEA FILE=HCAPLUS ABB=ON PLU=ON L30 NOT (L1 OR L3)

=>

=> d ibib abs hitstr 135 1

L35 ANSWER 1 OF 1 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:42245 HCAPLUS

DOCUMENT NUMBER: 138:106689

TITLE: Preparation of thiazolylamino benzamide derivatives as

modulators of cell proliferation and inhibitors of

protein kinases

INVENTOR(S): Chu, Shao Song; Alegria, Larry Andrew; Bleckman, Ted

Michael; Chong, Wesley K. M.; Duvadie, Rohit K.; Li,

Lin; Reich, Siegfried H.; Romines, William H.;

Wallace, Michael B.; Yang, Yi

PATENT ASSIGNEE(S): Agouron Pharmaceuticals, Inc., USA

SOURCE: PCT Int. Appl., 163 pp. CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

		APPLICATION NO.	DATE				
WO 2003004467 WO 2003004467	A2 20030116	WO 2002-US21280	20020705				
		BA, BB, BG, BR, BY,	BZ. CA. CH. CN				
		DZ, EC, EE, ES, FI,					
		JP, KE, KG, KP, KR,					
		MK, MN, MW, MX, MZ,					
		SI, SK, SL, TJ, TM,					
	UZ, VN, YU, ZA,		IN, IR, II, IZ,				
		•	761 AM AZ DV				
		SL, SZ, TZ, UG, ZM,					
		BE, BG, CH, CY, CZ,					
		MC, NL, PT, SE, SK,					
		ML, MR, NE, SN, TD,					
CA 2452609		CA 2002-2452609					
		US 2002-190219	20020705				
US 6720346							
EP 1438046	A2 20040721	EP 2002-782499	20020705				
R: AT, BE, CH,	DE, DK, ES, FR,	GB, GR, IT, LI, LU,	NL, SE, MC, PT,				
IE, SI, LT,	LV, FI, RO, MK,	CY, AL, TR, BG, CZ,	EE, SK				
JP 2005521631	T2 20050721	JP 2003-510635	20020705				
PRIORITY APPLN. INFO.:		US 2001-303679P	P 20010706				
		US 2001-305274P	P 20010713				
		WO 2002-US21280	W 20020705				
OTUED COMPCE/C).	MADDAT 120.1066						

OTHER SOURCE(S): MARPAT 138:106689

$$R^{1}R^{2}N$$
  $C$   $NH_{2}$   $C$   $C$   $O$   $R^{3}$   $NH_{2}$   $C$   $O$   $R^{3}$ 

AB Aminothiazole compds. with mono-/di-substituted benzamides (shown as I; variables described below; e.g. 4-[[4-amino-5-(2,6-difluorobenzoyl)thiazol-2-yl]amino]-N-(2-morpholin-4-ylethyl)benzamide), and their pharmaceutically acceptable salts, pharmaceutically acceptable prodrugs,

Ι

pharmaceutically active metabolites, and pharmaceutically acceptable salts of said metabolites are described. These agents modulate and/or inhibit the cell proliferation and activity of protein kinases and are useful as pharmaceuticals for treating malignancies and other disorders. Inhibitory activities towards three cyclin complexes of protein kinases, phosphorylated FGF receptor and/or LCK tyrosine kinase and/or cytotoxicity towards the HCT-116 cancer cell line are reported for hundreds of I, many of which were prepared combinatorially. For I: R1 and R2 are each independently H, or an alkyl, alkenyl, alkynyl, heteroalkyl, alkoxy, aminoalkyl, aryl, heteroaryl, cycloalkyl, or heterocycloalkyl group unsubstituted or substituted with ≥1 substituents listed in the claims, or R1 or R2, together with the N-C(O) and two adjacent C atoms of the Ph ring of I, forms a 5- or 6-membered ring structure fused to the Ph ring of I and unsubstituted or substituted with ≥1 substituents listed in the claims, or R1 and R2, taken together with the N atom to which they are bonded, form a monocyclic or fused or nonfused polycyclic structure which may contain 1-3 addnl. heteroatoms, the structure being unsubstituted or substituted with ≥1 substituents listed in the claims. R3 is an aryl, heteroaryl, alkyl, or cycloalkyl group, unsubstituted or substituted with ≥1 substituents listed in the claims. Y is H, alkyl, heteroalkyl, haloalkyl, halocycloalkyl, haloheterocycloalkyl, cycloalkyl, heterocycloalkyl, -NO2, -NH2, -N-OH, N-ORC, -CN, -(CH2)z-CN (z is 0-4), halogen, -OH, -O-Ra-O-, -ORb, -CO-R, -O-CO-Rc, -O-CO-OR, -O-CO-OR, -O-OR, =O, =S, -NRdRe, -CO-NRdRe, -O-CO-NRdRe, -NRc-CO-Re, -NR-CO-OR, -CO-NRc-CO-Rd, -O-SO2-Re, -O-SO-R, -O-S-Re, -S-CO-Rc, -SO-CO-ORc, -SO-CO-OR, -O-SO3, -NRc-SRd, -NRc-SO-Rd,  $\label{eq:nrc-so2-rd} $$NRc-SO2-Rd$, -CO-SRc$, -CO-SO-Re$, -CO-OSO2-Rc$, -CS-Rc$, -CSO-R$, -CSO2-R$, -NRc-CS-Rd$, -O-CS-Re$, -O-CSO-Rc$, -O-SO2-Re$, -OS2-NRdRe$, -SO-NRdRe$,$ -S-NRdRe, -NRd-CSO2-Rd, - NRc-CSO-Rd, -NRc-CS-Rd, -SH, -S-Rb, and -PO2-ORc (Ra, etc. defined in claims). Although the methods of preparation are not claimed, .apprx.80 example prepns. of I are included and directions are given for combinatorial preparation of 396 I.

IT 486415-56-9P, 3-[[4-Amino-5-(2,6-difluorobenzoyl)thiazol-2yl]amino]-N-(2-methylaminoethyl)benzamide
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES
(Uses)

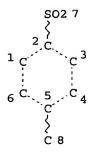
(drug candidate; preparation of thiazolylamino benzamide derivs. as modulators of cell proliferation and inhibitors of protein kinases) 486415-56-9 HCAPLUS

Benzamide, 3-[[4-amino-5-(2,6-difluorobenzoy1)-2-thiazoly1]amino]-N-[2-(methylamino)ethyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O \\ \parallel \\ NH - CH_2 - CH_2 - NH - C \\ \hline \\ C = O \\ \hline \\ F \end{array}$$

RN CN

=> => d stat que STR L13



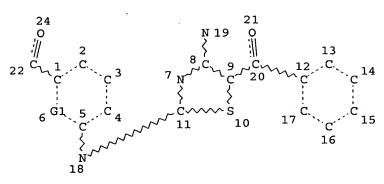
NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC 1

NUMBER OF NODES IS

STEREO ATTRIBUTES: NONE L15 STR



VAR G1=C/N NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

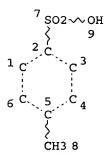
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 23

STEREO ATTRIBUTES: NONE

L18 365356 SEA FILE=REGISTRY SSS FUL L13 OR L15

L21 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

**GRAPH ATTRIBUTES:** 

RSPEC 1

NUMBER OF NODES IS 9

STEREO ATTRIBUTES: NONE

L23 STR

 $N \sim CH2 \cdot CH \sim NH2$ 1 2 3 4

NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE

L24 65 SEA FILE=REGISTRY SUB=L18 SSS FUL L21 AND L23

L36 45 SEA FILE=HCAPLUS ABB=ON PLU=ON L24/P

L37 39 SEA FILE=HCAPLUS ABB=ON PLU=ON L36 AND PD=<NOVEMBER 5, 2003

=>

-

=> d ibib abs hitstr 137 1-39

L37 ANSWER 1 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:162463 HCAPLUS

DOCUMENT NUMBER: 140:217642

TITLE: Preparation of spiro- and dispiro-1,2,4-trioxolanes as

antimalarial agents, schistosomicides, and anticancer

agents

INVENTOR(S): Vennerstrom, Jonathan L.; Dong, Yuxiang; Chollet,

Jacques; Matile, Hugues; Padmanilayam, Maniyan; Tang,

Yuanqing; Charman, William N.

PATENT ASSIGNEE(S): Medicines for Malaria Venture MMV, Switz.

SOURCE: U.S. Pat. Appl. Publ., 75 pp., Cont.-in-part of Appl.

No. PCT/US02/19767.

CODEN: USXXCO

DOCUMENT TYPE: Patent

LANGUAGE:

GΙ

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PA'	PATENT NO.						KIND DATE			APPLICATION NO.										
	US 6825230					A1 20040226 B2 20041130			US 2003-642721											
WO	2003	0006	76		A1		2003	0103	1	WO 2	002-	US19		20020621 <						
	W :	ΑE,	AG,	AL,	AM,	AT,	ΑU,	AZ,	BA,	BB,	BG,	BR,	BY,	BZ,	CA,	CH,	CN,			
		CO,	CR,	CU,	CZ,	DE,	DK,	DM,	DZ,	EE,	ES,	FI,	GB,	GD,	GE,	GH,	GM,			
		HR,	HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	KZ,	LC,	LK,	LR,	LS,			
		LT,	LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	ΜZ,	NO,	NZ,	PL,	PT,	RO,			
		RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	TZ,	UA,	UG,	US,	UZ,			
		VN,	YU,	ZA,	ZW,	AM,	AZ,	BY,	KG,	KZ,	MD,	RU,	ТJ,	TM						
	RW:	GH,	GM,	KΕ,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZM,	ZW,	ΑT,	BE,	CH,			
		CY,	DE,	DK,	ES,	FΙ,	FR,	GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	PT,	SE,	TR,			
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	GQ,	GW,	ML,	MR,	NE,	SN,	TD,	TG			
SG	1095	59			A1		2005	0330		SG 2	004-	4498			2	0040	303			
EP	1514	871			A1		2005	0316		EP 2	004-	2548	21		2	0040	311			
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	IT,	LI,	LU,	NL,	SE,	MC,	PT,			
		ΙE,	SI,	LT,	LV,	FI,	RO,	MK,	CY,	AL,	TR,	BG,	CZ,	EE,	HU,	PL,	SK, HR	₹		
JP	JP 2005060396				A2		2005	0310		JP 2	004-	2363	04		2	0040	316			
PRIORIT	PRIORITY APPLN. INFO.:							WO 2002-US19767					A2 20020621							
								US 2001-886666					A 20010621							
									US 2003-642721					A 20030818						
OTHER SOURCE(S):					MARPAT 140:21764				42											

$$X \stackrel{O-O}{\underset{R^2}{\bigvee}} X \stackrel{R^1}{\underset{R^2}{\bigvee}} 0 \stackrel{O-O}{\underset{N-SO_2-Bu}{\bigvee}} 1$$

$$N-OMe$$
 III  $O$  IV

Spiro and dispiro 1,2,4-trioxolanes of formula I [wherein: R1 and R2 are AΒ the same or different, and are selected from the group consisting of H, (un) substituted linear or branched alkyl aryl, alkaryl, and alicyclic groups, etc.; X = C or N] were prepared as antimalarial agents and schistosomicides. Claims cover these uses (prophylaxis and treatment) as well as use in the treatment of cancer (no data). Over 240 synthetic examples are disclosed. Trioxolanes I were screened against (1) chloroquine-resistant K1 and chloroquine-sensitive NF54 strains of Plasmodium falciparum in vitro, (2) Schistosoma mansoni in vivo (mice

infected), and (3) P. berghei. Antimalarial activity of I falls off when the trioxolane peroxide bond is too exposed or is sterically inaccessible to Fe(II) species; other factors influencing an antimalarial activity include the stability of carbon radicals formed by  $\beta$ -scission subsequent to the initial electron transfer to the peroxide bond and the influence of steric effects remote from the peroxide bond on the interactions between carbon radicals and potential drug target. For instance, compound II (i.e., I; X = N, R1 = SO2C4H9, no R2; IC50 = 1.6/0.4 ng/mL for K1/NF54) was prepared via reaction of O-Me 2-adamantanone oxime (III), cyclohexanone derivative IV, and ozone with the yield of 36%. 664338-76-5P

RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of spiro/dispiro-1,2,4-trioxolanes useful as antimalarial agents and schistosomicides)

RN 664338-76-5 HCAPLUS

Dispiro[cyclohexane-1,3'-[1,2,4]trioxolane-5',2''tricyclo[3.3.1.13,7]decane]-4-acetamide, N-(2-aminoethyl)-, cis-,
mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

IT

CN

CRN 664338-75-4 CMF C20 H32 N2 O4

Relative stereochemistry.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

REFERENCE COUNT: 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 2 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:17437 HCAPLUS

DOCUMENT NUMBER: 132:166176

TITLE: Reactions of 3-amino-1-phenyl- and

3-amino-1-(2-thienyl)-4,4,4-trifluorobut-2-en-1-ones

with 1,2-diaminopropane and 1,2-diamino-3,3,3-

trifluoropropane

AUTHOR(S): Sosnovskikh, V. Ya.; Kutsenko, V. A.; Aizikovich, A.

Ya.; Korotaev, V. Yu.

CORPORATE SOURCE: A. M. Gorky Ural State University, Yekaterinburg,

620083, Russia

SOURCE: Russian Chemical Bulletin (Translation of Izvestiya

Akademii Nauk, Seriya Khimicheskaya) (1999),

48(11), 2112-2116

CODEN: RCBUEY; ISSN: 1066-5285

PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal LANGUAGE: English

AB The reactions of 3-amino-1-phenyl- and 3-amino-1-(2-thienyl)-4,4,4-trifluorobut-2-en-1-ones with 1,2-diaminopropane under kinetically controlled conditions afford mixts. of cis and trans isomers of 2-aroylmethyl-4-methyl-2-trifluoromethylimidazolidines. Analogous

reactions with 1,2-diamino-3,3,3-trifluoropropane yield cis-2-aroylmethyl-2,4-bis(trifluoromethyl)imidazolidines.

IT 259138-26-6P

259138-26-6 HCAPLUS

CN 1,2-Propanediamine, 3,3,3-trifluoro-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

RN

CRN 259138-23-3 CMF C3 H7 F3 N2

NH<sub>2</sub> | H<sub>2</sub>N- CH<sub>2</sub>- CH- CF<sub>3</sub>

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

HO3S Me

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 3 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:640828 HCAPLUS

DOCUMENT NUMBER: 131:272178

TITLE: Preparation of N-(mercaptoalkyl)urea derivatives of

amino acids as inhibitors of  $TNF-\alpha$  production

INVENTOR(S): Mita, Shiro; Horiuchi, Masato; Ban, Masakazu; Suhara,

Hiroshi

PATENT ASSIGNEE(S): Santen Pharmaceutical Co., Ltd., Japan

SOURCE: PCT Int. Appl., 324 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.						KIND DATE			APPLICATION NO.						DATE			
									-						-				
	WO	9950	238			A1		1999	1007	V	O	1999-	JP15	54		1	9990	325	<
		W :	CA,	CN,	KR,	NO,	US												
		RW:	AT,	BE,	CH,	CY,	DE,	DK,	ES,	FI,	FR	, GB,	GR,	ΙE,	IT,	LU,	MC,	NL,	
			PT,	SE															
	JΡ	2000	0445	33		A2		2000	0215	ن	JΡ	1999-	7834	6		1	9990	323	<
	JP	3603	177			B2		2004	1222										
	CA	2325	741			AA		1999	1007		CA	1999-	2325	741		1	9990	325	<
	EP	1072	591			A1		2001	0131	E	ΞP	1999-	9107	24		1	9990	325	<
		R:	AT,	BE,	CH,	DE,	DK,	, ES,	FR,	GB,	GR	, IT,	LI,	LU,	NL,	SE,	MC,	PT,	
			ΙE,	FI															
	US	6492	370			B1		2002	1210	τ	JS :	2000-	6237	79		2	0000	908	<
	US	2002	1983	76		A1		2002	1226	τ	JS :	2002-	1471	31		2	0020	515	<
	US	6730	784			B2		2004	0504										
PRIO	RITY	APP	LN.	INFO	. :					ت	JP	1998-	7915	4	7	A 1	.9980	326	
										V	10	1999-	JP15	54	1	<i>N</i> 1	.9990	325	
										τ	JS :	2000-	6237	79	7	A3 2	0000	908	
OTHE	ס פר	מססוור	/cl.			MADI	ידי עכו	121.	2721	70									

OTHER SOURCE(S): MARPAT 131:272178

GI

$$\begin{array}{c|c} & & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

AB Prepared are α-[N'-(mercaptoalkyl)ureido]alkanamide compds. having a urea structure as the basic structure and carrying sulfur and amide bonds in side chains. The above compds. are represented by general formula R1S-A1(R7)-NR2CONR3-A2(R4)CONR5R6 [wherein R1 represents H, (un)substituted lower alkyl or aromatic group, RA-CO-, RC-S- or a group of formula S-A1(R7)-NR2CONR3-A2(R4)CONR5R6; R2, R3 and R4 represent each H, (un)substituted lower alkyl or alkenyl, cycloalkyl, cycloalkenyl or (un)substituted aromatic group; R5 and R6 represent each H, (un)substituted lower alkyl or alkenyl, cycloalkyl, cycloalkenyl or (un)substituted aromatic group, or R5 and R6 may form together (un)substituted nonarom. heterocycle; R7 represents H, (un)substituted lower alkyl, cycloalkyl, hydroxy, mercapto, Ph, RB-O-, RC-S-, RD-COS-, RE-OCO-, RF-N(RG)- or -CONHOH; A1 and A2 represent each an alkylene; RA represents lower

(halo)alkyl, aromatic group, lower alkoxy, aromatic-lower alkoxy, RF, or NRG; RB

represents lower alkyl or aromatic group; RC represents H, lower alkyl, aromatic

group; RD represents lower alkyl or aromatic group; RE represents H, lower alkyl, or aromatic group, RF and RG represent H, lower alkyl, cycloalkyl, or aromatic group]. It has been found out that these compds. have pharmacol. effects, in particular, a tumor necrosis factor- $\alpha$  (TNF- $\alpha$ ) production inhibitory effect. They are useful as remedies for autoimmune diseases and as antirheumatics. Thus, (2S)-2-[3-[2-(acetylthio)ethyl]-3-(2-cyclohexylethyl)ureido] propionic acid (preparation given) was condensed with N-methylpiperazine using 1-hydroxybenzotriazole, 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride, and N-methylmorpholine in CH2Cl2 at room temperature overnight to give the title compound (I; X = NMe) in 78% yield. I (X = NMe) and I (X = 0) at 50 mg/kg p.o. inhibited the Salmonella lipopolysaccharide-induced production of TNF- $\alpha$  in rats by 84.6 and 93.5%, resp.

IT 245487-21-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of N-(mercaptoalkyl)urea derivs. of amino acids as inhibitors of TNF- $\alpha$  production, antirheumatics, and remedies for autoimmune disease)

RN 245487-21-2 HCAPLUS

CN Alanine, 3-(dimethylamino)-, phenylmethyl ester, bis(4methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 245487-20-1 CMF C12 H18 N2 O2

$$\begin{array}{c|c} & \text{H}_2\text{N} & \text{O} \\ & | & || \\ \text{Me}_2\text{N}-\text{CH}_2-\text{CH}-\text{C}-\text{O}-\text{CH}_2-\text{Ph} \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 4 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:235587 HCAPLUS

DOCUMENT NUMBER: 130:337901

TITLE: The total synthesis of a technetium chelate-tamoxifen

complex

AUTHOR(S): Bell, Russell A.; Dickson, Kieran C.; Valliant, John

F.

CORPORATE SOURCE: Department of Chemistry, McMaster University,

Hamilton, ON, L8S 4M1, Can.

SOURCE: Canadian Journal of Chemistry (1999), 77(1),

146-154

CODEN: CJCHAG; ISSN: 0008-4042

PUBLISHER: National Research Council of Canada

DOCUMENT TYPE: Journal LANGUAGE: English

AB A potential agent for imaging breast cancer has been synthesized by derivatization of the anti-estrogen tamoxifen. A multistep synthesis was required to conjugate a technetium chelate to tamoxifen in such a fashion that the biodistribution of the complex should mimic that of the parent compound

IT 224184-30-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of tamoxifen-derived. chelate complex)

RN 224184-30-9 HCAPLUS

CN Alanine, 3-amino-, methyl ester, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 20610-20-2 CMF C4 H10 N2 O2

$$\begin{array}{c|c} \text{O} & \text{NH}_2 \\ \parallel & \parallel \\ \text{MeO-C-CH-CH}_2 - \text{NH}_2 \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

REFERENCE COUNT: 22 THERE ARE 22 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 5 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:42740 HCAPLUS

DOCUMENT NUMBER: 130:110060

TITLE: Preparation of hydroxycarbamoylalkylcarboxylic acid

hydrazides as inhibitors of tumor necrosis factor and

transforming growth factor release.

INVENTOR(S):
Broadhurst, Michael John; Johnson, William Henry;

Walter, Daryl Simon

PATENT ASSIGNEE(S): F. Hoffmann-La Roche A.-G., Switz.

SOURCE: Ger. Offen., 64 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KINI	D DATE	APPLICATION NO.	
			DE 1998-19829229	
US 6235787	B1	20010522	US 1998-98235	19980616 <
CA 2295062	AA	19990114	CA 1998-2295062	19980618 <
WO 9901428	A1	19990114	CA 1998-2295062 WO 1998-EP3683	19980618 <
			BG, BR, BY, CA, CH,	
			GM, GW, HU, ID, IL,	
			LT, LU, LV, MD, MG,	
			SE, SG, SI, SK, SL,	
			AZ, BY, KG, KZ, MD,	
			UG, ZW, AT, BE, CH,	
			MC, NL, PT, SE, BF,	
		MR, NE, SN,		20, 61, 63, 61,
AU 9886273	A1	19990125	AU 1998-86273	19980618 <
	B2	20001005	1330 00273	13300010 (
EP 993442	A1	20000419	EP 1998-937498	19980618 <
EP 993442	B1	20030423	EP 1998-937498	25500020
			GB, GR, IT, LI, LU,	
	SI, LT, LV,			, , , , , , , , , , , , , , , , , , , ,
TR 9903281	T2		TR 1999-9903281	19980618 <
BR 9810952	Α		BR 1998-10952	
JP 200051375	0 T2	20001017	JP 1999-506230	19980618 <
AT 238277	E	20030515		19980618 <
PT 993442	${f T}$	20030930	PT 1998-937498	19980618 <
ES 2195365	E T T3 A B1	20031201		19980618
ZA 9805469	A	19981230	ZA 1998-5469	19980623 <
IT 1301792	B1	19981230 20000707	IT 1998-MI1441	19980623 < 19980624 <
FR 2765219	A1	19981231	FR 1998-8124	19980626 <
FR 2765219	B1	19991029		
	A1	19990106		19980629 <
ES 2140348	Al	20000216	ES 1998-1359	19980629 <
ES 2140348	B1	20001016		
MX 9911668				19991214 <
BG 104050	Α		BG 1999-104050	19991228 <
NO 9906534	Α	20000223	NO 1999-6534	19991228 < 19991229 <
PRIORITY APPLN. II	NFO.:		GB 1997-13833	A 19970630
			GB 1997-13833 GB 1998-3335 WO 1998-EP3683	A 19980217
			WO 1998-EP3683	W 19980618

OTHER SOURCE(S):

AB Title compds. [I; Y = CO, SO2; R1 = alkyl, alkenyl, cycloalkyl, cycloalkylalkyl, aryl, aralkyl; R2 = alkyl, haloalkyl, aralkyl, aralkenyl,

MARPAT 130:110060

aryl, alkoxy, alkoxycarbonyl, etc.; R3 = H, (substituted) alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkylalkyl, aralkyl, aralkenyl, aryl, heterocyclyl; R2R3 = 5-7 membered cyclic amide, imide, sulfonamide, or urethane; R4 = alkyl, alkenyl, cycloalkylalkyl, ArX, HetX, etc.; Ar = aryl; Het = heteroaryl; X = spacer], were prepared Thus, (E)-2(R)-[1(S)-(hydroxycarbamoyl)-4-phenyl-3-butenyl]-2'-(methanesulfonyl)-4-methyl-2'-phenylvalerohydrazide (multistep preparation given) inhibited TNF $\alpha$  and TGF $\alpha$  release with IC50 = 437 nM and 210 nM, resp.

IT 219613-60-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of hydroxycarbamoylalkylcarboxylic acid hydrazides as inhibitors of tumor necrosis factor and transforming growth factor release)

RN 219613-60-2 HCAPLUS

CN 5-Hexenoic acid, 3-[(hydroxyamino)carbonyl]-2-(2-methylpropyl)-6-phenyl-,
2-(2-aminoethyl)-2-(methylsulfonyl)hydrazide, (2R,3S,5E)-,
mono(4-methylbenzenesulfonate) (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 219613-59-9 CMF C20 H32 N4 O5 S

Absolute stereochemistry.

Double bond geometry as shown.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 6 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:411171 HCAPLUS

DOCUMENT NUMBER: 129:109388

TITLE: Inclusional Complexation by Cyclodextrin-Polymer

Hoffman 10\_631358 Conjugates in Organic Solvents AUTHOR (S): Hirasawa; Takuro; Maeda, Yasushi; Kitano, Hiromi Department of Chemical and Biochemical Engineering, CORPORATE SOURCE: Toyama University, Toyama, 930-8555, Japan Macromolecules (1998), 31(14), 4480-4485 CODEN: MAMOBX; ISSN: 0024-9297 SOURCE: PUBLISHER: American Chemical Society DOCUMENT TYPE: Journal LANGUAGE: English  $\beta$ -Cyclodextrin ( $\beta$ -CD) was modified with poly(Nisopropylacrylamide) (PIPA, Mn = 2.5 + 103) or poly(ethylene glycol) (PEG, Mn = 5.15 + 103) chains (PIPA- $\beta$ -CD or PEG- $\beta$ -CD, resp.). In aqueous solns. of PIPA- $\beta$ -CD and PEG- $\beta$ -CD, an inclusion of 2-anilino-6-naphthalenesulfonic acid (2,6-ANS) into a cavity of the modified cyclodextrin increased the fluorescence intensity similarly to a free  $\beta$ -CD-2,6-ANS system. The association consts. for 2,6-ANS-PIPA- $\beta$ -CD and 2,6-ANS-PEG- $\beta$ -CD systems evaluated were, however, slightly smaller than that for the free  $\beta$ -CD-2,6-ANS system, due to a steric hindrance by the polymer chains on the rim of CD. The PIPA- $\beta$ -CD and PEG- $\beta$ -CD could be easily dissolved in a tetrahydrofuran-phosphate buffer (M/30, pH 7.2) mixture (99:1), and the fluorescence intensity of 2,6-ANS in this medium was decreased by the presence of PIPA- $\beta$ -CD and PEG- $\beta$ -CD. A similar tendency was observed in the case of PEG-β-CD dissolved in a 1,4-dioxane-buffer mixture (99:1). This phenomenon might be attributed to the inclusion of 2,6-ANS in the less nonpolar environment of the cavity of CD-polymer conjugates than that of bulk solution (tetrahydrofuran-buffer and 1,4-dioxane-buffer, 99:1), which is consistent with the fact that the peak positions of both fluorescence spectra of 2,6-ANS and 8-anilino-1-naphthalenesulfonic acid (1,8-ANS) and electronic spectra of p-tert-butylphenol in aqueous  $\beta$ -CD solution were similar to those in polar organic solvents such as glycerol. 209996-87-2DP, polymer complexes, inclusion compds. with ΙT anilinonaphthalenesulfonic acid RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (inclusional complexation by cyclodextrin-polymer conjugates in organic solvents and properties of the resulting compds.) 209996-87-2 HCAPLUS RN β-Cyclodextrin, 4-methylbenzenesulfonate, compd. with CN 1,2-ethanediamine (9CI) (CA INDEX NAME) CM CRN 107-15-3 CMF C2 H8 N2  $H_2N-CH_2-CH_2-NH_2$ CM 2 CRN 187284-10-2 CMF C42 H70 O35 . x C7 H8 O3 S

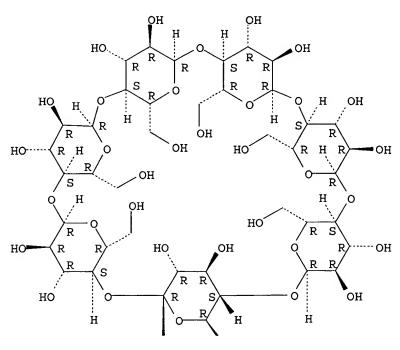
> CRN 7585-39-9 CMF C42 H70 O35

3

CM

Absolute stereochemistry.

PAGE 1-A



PAGE 2-A

CM 4

CRN 104-15-4

CMF C7 H8 O3 S

IT 209996-87-2P

CN

RL: SPN (Synthetic preparation); PREP (Preparation) (inclusional complexation by cyclodextrin-polymer conjugates in organic solvents and properties of the resulting compds.)

RN 209996-87-2 HCAPLUS

 $\beta$ -Cyclodextrin, 4-methylbenzenesulfonate, compd. with 1,2-ethanediamine (9CI) (CA INDEX NAME)

CM 1

CRN 107-15-3 CMF C2 H8 N2

 $_{\rm H_2N^-\,CH_2^-\,CH_2^-\,NH_2}$ 

CM 2

CRN 187284-10-2 CMF C42 H70 O35 . x C7 H8 O3 S

CM 3

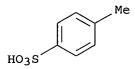
CRN 7585-39-9 CMF C42 H70 O35

Absolute stereochemistry.

PAGE 1-A

CM 4

CRN 104-15-4 CMF C7 H8 O3 S



REFERENCE COUNT: 54 THERE ARE 54 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 7 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:532510 HCAPLUS

DOCUMENT NUMBER: 127:149109

TITLE: Azino-Fused Benzimidazolium Salts as DNA Intercalating

Agents. 2.

AUTHOR(S): Pastor, Joaquin; Siro, Jorge G.; Garcia-Navio, Jose

L.; Vaquero, Juan J.; Alvarez-Builla, Julio; Gago, Federico; de Pascual-Teresa, Beatriz; Pastor, Manuel;

Rodrigo, M. Melia

CORPORATE SOURCE: Departamento de Quimica Organica Departamento de

Quimica-Fisica and Departamento de Farmacologia,

Universidad de Alcala, Madrid, 28871, Spain

SOURCE: Journal of Organic Chemistry (1997), 62(16),

5476-5483

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB The synthesis of new pyrido[1,2-a] - and pyridazino[1,6-a]benzimidazolium

salts by basic condensation of 1,3-disubstituted 2-alkylbenzimidazolium salts and 1,2-diketones and subsequent chemical transformations is described.

The DNA-binding properties were examined by UV-vis spectroscopy,

viscosimetric determination, and mol. modeling techniques. The presence of a

flat

polycyclic hydrocarbon moiety such as a naphthalene-1,8-diyl or a biphenyl-o,o'-diyl, fused to the cationic heterocycle, appears to enhance the interaction with DNA. Variation of the substituents on the indole-like N will allow us to build up a new series of bis-salts with bis-intercalating properties.

IT 174146-38-4P

RL: BSU (Biological study, unclassified); PEP (Physical, engineering or chemical process); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation); PROC (Process)

(preparation of azino-fused benzimidazolium salts as DNA intercalating agents)

RN 174146-38-4 HCAPLUS

CN Acenaphtho[1',2':3,4]pyridazino[1,6-a]benzimidazolium,
13-[2-[(2-aminoethyl)amino]-2-oxoethyl]-, salt with 2,4,6trimethylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 174146-37-3

### CMF C24 H20 N5 O

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{H}_2\text{N}-\text{CH}_2-\text{CH}_2-\text{NH}-\text{C}-\text{CH}_2 \\ & & & \\ & &$$

CM 2

CRN 46149-61-5 CMF C9 H11 O3 S

GI

L37 ANSWER 8 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:335195 HCAPLUS

DOCUMENT NUMBER: 127:5342

TITLE: Flexible and Convergent Total Synthesis of

Cyclotheonamide B

AUTHOR(S): Bastiaans, Harold M. M.; van der Baan, Juul L.;

Ottenheijm, Harry C. J.

CORPORATE SOURCE: Leiden/Amsterdam Center for Drug Research Division of

Medicinal Chemistry Department of Pharmacochemistry,

Vrije Universiteit, Amsterdam, Neth.

SOURCE: Journal of Organic Chemistry (1997), 62(12),

3880-3889

CODEN: JOCEAH; ISSN: 0022-3263

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 127:5342

AB A convergent approach using two key intermediates, tripeptide segment A
(I) and dipeptide segment B (II), was developed for the synthesis of
cyclotheonamide B. The starting compound for the preparation of the
homoarginine

(hArg) moiety, the predominant part of segment A, was Z-Arg(Boc)2-OMe (Z = PhCH2O2C; Boc = Me3CO2C), which was converted into the corresponding aldehyde and subsequently homologated using (MeS) 3CLi as a carboxylic acid anion equivalent Coupling with properly protected Pro and D-Phe derivs. gave smoothly the desired Pro-hArg-D-Phe tripeptide derivative The key feature of segment B, i.e., the L-tyrosine-derived  $\alpha,\beta$ -unsatd.  $\gamma$ -amino acid, was prepared by a Wadsworth-Emmons olefination of the aldehyde derived from Boc-Tyr(CMe3)-OMe. Selective N-Boc removal in the presence of the aryl tert-Bu ether present in the fully protected segment B was achieved by treatment with trimethylsilyl triflate/2,6-lutidine to give the vinylogous Tyr-Dpr dipeptide ester in quant. yield. Coupling of the key intermediates using TBTU afforded the fully protected linear pentapeptide in high yield. Treatment of the fully protected linear pentapeptide with Pd(PPh3)4/morpholine resulted in simultaneous removal of the C-terminal allyl group and the N-terminal allyloxycarbonyl group, which was then cyclized under dilution conditions by treatment with TBTU/HOBt/DMAP to give the protected cyclopentapeptide in 61% yield. Oxidation of the hydroxyl group with Dess-Martin periodinane in the presence of tert-Bu alc. gave the corresponding oxo amide, which was then subjected to O,N-deprotection with CF3CO2H/thioanisole. Subsequent HPLC purification afforded cyclotheonamide B in an overall yield of 1.8% in 17 steps.

IT 190203-22-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(flexible and convergent total synthesis of cyclotheonamide B)

RN 190203-22-6 HCAPLUS

CN L-Alanine, 3-amino-, 2-propenyl ester, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 171109-52-7 CMF C6 H12 N2 O2

Absolute stereochemistry. Rotation (+).

CM

CRN 104-15-4 CMF C7 H8 O3 S

REFERENCE COUNT: 40 THERE ARE 40 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 9 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

1997:122435 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 126:157906

TITLE: Terminal modification of Nylon 6 by the reaction of

diamine/sulfonic acid salts

AUTHOR (S): Sasaki, Akio; Kimura, Yoshiharu

CORPORATE SOURCE: Technical Dev. Div., Unitika Ltd., Osaka, 541, Japan

SOURCE: Nippon Kagaku Kaishi (1997), (2), 153-158

CODEN: NKAKB8; ISSN: 0369-4577

PUBLISHER: Nippon Kaqakkai

DOCUMENT TYPE: Journal LANGUAGE: Japanese

Several diamine/acid salts were reacted with Nylon 6 in melt state to

increase ammonium terminal groups in Nylon 6. 1,6-

Diaminohexane/methanesulfonic acid (1:2) salt was the most effective for this terminal modification. When its molar ratio was 1.2 relative to the terminal carboxyl groups of Nylon 6, a significant amount of the ammonium-sulfonate groups were introduced without decreasing the solution viscosity of polymer. Model reactions revealed that the diamine/acid salts can react with the terminal carboxyl groups or the inner amide groups of Nylon 6 to form the ammonium terminal groups. The same terminal

modification was possible when the diamine salts were added to the

polymerization

system of  $\epsilon$ -caprolactam. The reaction product of Nylon 6 and 1,6-diaminohexane/methanesulfonic acid (1:2) salt was melt-spun into a filament. Its dyeability to acidic dye was very high even in a neutral bath because of increased ammonium terminal groups. This filament was then mixed with the formerly prepared s-triazine-terminated filaments and the original Nylon 6 filament, and the filament mixture was dyed in a mixed bath containing both acidic and basic dyes for cross dyeing. Each of the filaments was dyed with the corresponding dyes sep. This technique should be economically useful in dyeing industry and can be applied to the industrial production of new functional Nylon fiber or plastics.

IT 23571-07-5DP, p-Toluenesulfonic acid, 1,2-diaminoethane (2:1)

salt, reaction products with nylon 6

RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation) (terminal modification of nylon 6 by reaction with diamine/sulfonic acid salts)

RN 23571-07-5 HCAPLUS

CN 1,2-Ethanediamine, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 107-15-3 CMF C2 H8 N2

 $H_2N-CH_2-CH_2-NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

HO3S Me

L37 ANSWER 10 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:10649 HCAPLUS

DOCUMENT NUMBER: 124:202184

TITLE: Synthesis of new azino fused benzimidazolium salts. A

new family of DNA intercalating agents. I

AUTHOR(S): Pastor. Joaquin; Siro, Jorge; Garcia-Navio, Jose L.;

Vaquero, Juan J.; Rodrigo, M. Melia; Ballesteros,

Milagros; Alvarez-Builla, Julio

CORPORATE SOURCE: Dep. Quim. Org., Univ. Alcala de Henares, Alcala de

Henares, 28871, Spain

SOURCE: Bioorganic & Medicinal Chemistry Letters (1995

), 5(24), 3043-8

CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of new pyrido[1,2-a]benzimidazolium salts and pyridazino[1,6-a]benzimidazolium salts was prepared from readily available 1,3-disubstituted 2-alkylbenzimidazolium salts. Their affinity to DNA and in vitro cytotoxicity vs. HT-29 (colon carcinoma) have been tested. The initial results show that the title compds. are a new family of intercalating agents.

IT 174146-38-4P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)

(preparation and activity of pyridobenzimidazolium salts and pyridazinobenzimidazolium salts as DNA intercalating agents)

RN 174146-38-4 HCAPLUS

CN Acenaphtho[1',2':3,4]pyridazino[1,6-a]benzimidazolium, 13-[2-[(2-aminoethyl)amino]-2-oxoethyl]-, salt with 2,4,6trimethylbenzenesulfonic acid (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 174146-37-3 CMF C24 H20 N5 O

CM 2

CRN 46149-61-5 CMF C9 H11 O3 S

L37 ANSWER 11 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:478277 HCAPLUS

DOCUMENT NUMBER: 122:216579

TITLE: Reactive dyes and manufacture and use thereof

PATENT ASSIGNEE(S): Ciba-Geigy A.-G., Switz.

SOURCE: Jpn. Kokai Tokkyo Koho, 35 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
				-	
JP 06329938	A2	19941129	JP 1994-125889		19940517 <
US 5684138	Α	19971104	US 1996-657455		19960529 <
PRIORITY APPLN. INFO.:			CH 1994-1494	Α	19930517
			CH 1993-1950	Α	19930629
			CH 1993-1494	Α	19930517
			US 1994-242514	A1	19940513

OTHER SOURCE(S): MARPAT 122:216579

GI

- \* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY AVAILABLE VIA OFFLINE PRINT \*
- AB Light- and wetfast reactive dyes have the general formula I [R1-4 = H, (un) substituted C1-4 alkyl; B = aliphatic linking group; Y1, Y2 = halogen, carboxypyridinium, etc.; A1 = substituent, e.g., Q (n = 0), etc.; A2 = substituent, e.g., Q (n = 1), etc.; R10 = C1-4 alkyl, alkoxy, halogen, carboxy, sulfo]. Cyanuric fluoride was condensed, sep., with 1-amino-4-(3-amino-2,4,6-trimethyl-5-sulfophenyl)anthraquinone-2-sulfonic acid and 5-amino-3-[3-phenyl-5-(2-carboxy-5-sulfophenyl)-1-formazano]-4-hydroxybenzenesulfonic acid copper complex, then the two reaction mixts. were combined and adjusted to pH 8.5 to give I (R1-4 = H; Y1 = Y2 = F; B = CH2CH2; A1 = Q1; A2 = Q2), bright blue on cotton.
- IT 162094-25-9P 162094-26-0P
  RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(in reactive dye manufacture)

RN 162094-25-9 HCAPLUS

CN 2-Anthracenesulfonic acid, 1-amino-4-[[3-[[4-[(2-aminoethyl)amino]-6-chloro-1,3,5-triazin-2-yl]amino]-2,4,6-trimethyl-5-sulfophenyl]amino]-9,10-dihydro-9,10-dioxo-(9CI) (CA INDEX NAME)

RN 162094-26-0 HCAPLUS

CN 2-Anthracenesulfonic acid, 1-amino-4-[[3-[[4-[(2-aminoethyl)amino]-6-fluoro-1,3,5-triazin-2-yl]amino]-2,4,6-trimethyl-5-sulfophenyl]amino]-9,10-dihydro-9,10-dioxo- (9CI) (CA INDEX NAME)

F N NH SO<sub>3</sub>H

$$H_2N-CH_2-CH_2-NH$$
 $HO_3S$ 
 $NH_2$ 
 $O$ 

L37 ANSWER 12 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:283587 HCAPLUS

DOCUMENT NUMBER: 122:229436

TITLE: Design and Synthesis of Calcium and Magnesium

Ionophores Based on Double-Armed Diazacrown Ether Compounds and Their Application to an Ion Sensing

Component for an Ion-Selective Electrode

AUTHOR(S): Suzuki, Koji; Watanabe, Kazuhiko; Matsumoto, Yukihiro;

Kobayashi, Mitsuru; Sato, Sayaka; Siswanta, Dwi;

Hisamoto, Hideaki

CORPORATE SOURCE: Department of Applied Chemistry, Keio University,

Yokohama, 223, Japan

SOURCE: Analytical Chemistry (1995), 67(2), 324-34

CODEN: ANCHAM; ISSN: 0003-2700

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal LANGUAGE: English

AB The double-armed diazacrown ethers, which have a base diazacrown ether ring with two diamide-type side chains, were designed and synthesized from the proposed mol. model for the novel neutral Ca2+ and Mg2+ ionophores. The potentiometric ion-selective electrodes were prepared with over 20 kinds of systematically synthesized diazacrown ether derivs. The relation between the mol. structures of the ionophores and the ion selectivities was fully discussed. The electrodes based on the 21- and 18-membered diazacrown ether derivs. possessing a glycolic diamide and malonic diamide in their side chains (K23E1 and K22B5) exhibited excellent Ca2+ and Mg2+ selectivities, resp. The ion-selectivity features of the novel Ca2+ and Mg2+ ionophores supply important structural information about the design of host mols. for alkaline earth metal cations.

IT 23571-07-5P, Ethylenediamine ditosylate

RL: PNU (Preparation, unclassified); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(for design and synthesis of calcium and magnesium ionophores based on double-armed diazacrown ether compds. and application to ion sensing component for ion-selective electrode)

RN 23571-07-5 HCAPLUS

CN 1,2-Ethanediamine, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 107-15-3

CMF C2 H8 N2

 $H_2N-CH_2-CH_2-NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

HO3S Me

L37 ANSWER 13 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:264514 HCAPLUS

DOCUMENT NUMBER: 122:56581

TITLE: Preparation of peptide analogs as inhibitors of

neutral endopeptidase and angiotensin converting

enzyme.

INVENTOR(S): Neustadt, Bernard R.; Smith, Elizabeth M.; Tulshian,

Deen

PATENT ASSIGNEE(S): Schering Corp., USA

SOURCE: PCT Int. Appl., 95 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	TENT :	NO.			KIN	) [	DATE		APP:	LICAT	ION	NO.		D	ATE	
													<b></b> -	-		
WO	9403	481			A1	1	1994	0217	WO	1993-	US71	37		1:	9930	803 <
	W:	AU,	BB,	BG,	BR,	BY,	CA,	CZ,	FI, HU	, JP,	KR,	KZ,	LK,	MG,	MN,	MW,
		NO,	ΝZ,	PL,	RO,	RU,	SD,	SK,	UA, US	, VN						
	RW:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, GR	, IE,	ΙT,	LU,	MC,	NL,	PT,	SE,
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN, ML	, MR,	ΝE,	SN,	TD,	TG		
US	5298	492			Α	1	1994	0329	US	1992-	9253	38		1	9920	804 <
AU	9347	919			A1	1	L994	0303	AU	1993-	4791	9		1.	9930	803 <
EP	6581	69			A1	1	1995	0621	EP	1993-	9184	88		1	9930	803 <
	R:	ΑT,	BE,	CH,	DE,	DK,	ES,	FR,	GB, GR	, IE,	IT,	LI,	LU,	MC,	NL,	PT, SE
JP	0750	9717			T2	1	1995	1026	JP	1993-	5054	32		1	9930	803 <
PRIORITY	Y APP	LN.	INFO	.:					US	1992-	9253	38	i	A2 1	9920	804
									WO	1993-	US71	37	1	W 1	9930	803

OTHER SOURCE(S): MARPAT 122:56581

GI

$$\begin{array}{c|c} & & & & \\ & & & & \\ \text{MeSO}_{2H} & & & & \\ & & & & \\ & & & & \\ & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\$$

AB Title compds. [I; Z = amino, alkylamino, dialkylamino, R9CONH, (substituted) guanidino; R1 = H, R7R8N; R2 = H, alkyl, cycloalkyl, arylalkyl, heteroarylalkyl; R3 = H, alkyl or cycloalkyl; R2R3C = 3-7 membered carbocyclic ring; R4 = H, alkyl, arylalkyl or heteroarylalkyl; R5, R6 = OH, alkoxy, amino, arylalkoxy, alkylamino, dialkylamino; R7 = R9CO, R10SO2; R8 = H, alkyl, arylalkyl, aryl; R7R8N = 5-7 membered ring; R9 = alkyl, arylalkyl, aryl, heteroarylalkyl, heteroaryl, alkoxy, arylalkoxy, amino, alkylamino, dialkylamino; R10 = alkyl, arylalkyl, aryl, heteroarylalkyl, amino, alkylamino, dialkylamino, heteroaryl; m, n = 1-5], were prepared Thus, title compound II (solution phase preparation given) inhibited

ACE with IC50 = 50 nM.

IT 159871-39-3P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for inhibitor of angiotensin converting enzyme and neutral endopeptidase)

RN 159871-39-3 HCAPLUS

CN L-Alanine, 3-[[(phenylmethoxy)carbonyl]amino]-, propyl ester, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 159871-38-2 CMF C14 H20 N2 O4

Absolute stereochemistry.

CM 2

CRN 104-15-4

### CMF C7 H8 O3 S

L37 ANSWER 14 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:193305 HCAPLUS

DOCUMENT NUMBER: 120:193305

TITLE: Acylamino group-containing copolymers and salt and

manufacture thereof and impact-resistant thermoplastic

resin compositions using the same

INVENTOR(S): Kitazawa, Naoki; Hotsuta, Hiroshi; Nakayama, Yutaka;

Sumi, Hideyuki

PATENT ASSIGNEE(S): Dai Ichi Kogyo Seiyaku Co Ltd, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 31 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 05279417	A2	19931026	JP 1992-80967	19920402 <
RIORITY APPLN. INFO.:			JP 1992-80967	19920402

PRIORITY APPLN. INFO.: JP 1992-80967 19920402

AB The title copolymers useful as compatibilizers for engineering plastics and polypropylene contain olefin (derivative)-based units and maleimide

(derivative) units having acyl group-containing substituent on the N-position.

An

impact-resistant composition comprised 70 parts Toughlon A2500, 30 parts polyethylene (Polyethy BV004), and 5 parts 90:5:5 ethylene-Et acrylate-maleic anhydride copolymer imidized by reaction product from N-(2-aminoethyl)piperazine and AcNMe2.

TT 7294-10-2DP, maleic anhydride copolymers imidized by amide compds. and 153429-41-5DP, maleic anhydride copolymers imidized by amide compds. and

RL: PREP (Preparation)

(manufacture of, for compatibilizers for engineering plastic-polyolefin blends)

RN 7294-10-2 HCAPLUS

CN 1,2-Ethanediamine, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 107-15-3 CMF C2 H8 N2

 $H_2N - CH_2 - CH_2 - NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 153429-41-5 HCAPLUS

CN 1,2-Ethanediamine, N-ethyl-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 110-72-5 CMF C4 H12 N2

EtNH-CH2-CH2-NH2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 15 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:135427 HCAPLUS

DOCUMENT NUMBER: 120:135427

TITLE: Copolymer having amino group and process for

production thereof

INVENTOR(S): Kitazawa, Naoki; Hotta, Hiroshi; Nakayama, Yutaka

PATENT ASSIGNEE(S): Daiichi Kogyo Seiyaku Co., Ltd., Japan

SOURCE: Eur. Pat. Appl., 74 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 558047	A2	19930901	EP 1993-103080	19930226 <
EP 558047	AZ A3	19931103	EP 1993-103080	19930226 (
EP 558047	B1	19980520		
R: BE, DE, FR,	GB, IT	, NL		
JP 05239134	A2	19930917	JP 1992-41860	19920228 <

JP 05239135 A2 19930917 JP 1992-41861 19920228 <--JP 05239136 A2 19930917 JP 1992-43972 19920228 <--JP 05239137 JP 1992-43973 A2 19930917 19920228 <--CA 2090563 AA 19930829 CA 1993-2090563 19930226 <--PRIORITY APPLN. INFO.: JP 1992-41860 Α 19920228 JP 1992-41861 A 19920228 JP 1992-43972 Α 19920228 JP 1992-43973 A 19920228

AB Polymers useful as high mol. weight amino reagents, raw materials for functional high polymers or additives, compatibilizers, curing agents, etc. are prepared by reaction of maleic anhydride (derivative)-containing polymers

with amino-containing salts or adducts.

IT 90747-78-7DP, reaction products with maleate (derivative)-containing

polymers

RL: PREP (Preparation) (preparation of) 90747-78-7 HCAPLUS

CN 1,2-Ethanediamine, N-ethyl-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

RN

CRN 110-72-5 CMF C4 H12 N2

EtNH-CH2-CH2-NH2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 16 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:604651 HCAPLUS

DOCUMENT NUMBER: 119:204651

TITLE: Compatible thermoplastic blends with low discoloration INVENTOR(S): Hotsuta, Hiroshi; Kitazawa, Naoki; Sugita, Yasuhisa;

Oota, Katsuhisa

PATENT ASSIGNEE(S): Idemitsu Petrochemical Co, Japan; Dai Ichi Kogyo

Seiyaku Co Ltd

SOURCE: Jpn. Kokai Tokkyo Koho, 32 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

JP 05032901 A2 19930209 JP 1991-191631 19910731 <-
PRIORITY APPLN. INFO.: JP 1991-191631 19910731

AP The title blends with good impact resistance comprise (A) 5-95%

The title blends with good impact resistance comprise (A) 5-95% thermoplastic polymers bearing groups reactive to amines, (B) 95-5% olefin and/or styrene polymers, and (C) 0.05-20 phr (of A + B) compatibilizers bearing units derived from vinyl compds., maleic acids modified with diamines and formyl-forming compds., etc. Thus, heating a maleic anhydride-styrene copolymer with an ethylenediamine p-toluenesulfonate-salt at reflux in xylene and DMF and detosylating gave a product bearing amine, formamide and imide groups. A blend containing the above product, a polycarbonate, and polypropylene gave test pieces without phase separation and good impact strength.

TT 7294-10-2DP, reaction products with maleated vinyl polymers,
modified to bear formamide groups

RL: PREP (Preparation)

(compatibilizing agents for thermoplastic blends, manufacture of)

RN 7294-10-2 HCAPLUS

CN 1,2-Ethanediamine, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 107-15-3 CMF C2 H8 N2

 $H_2N-CH_2-CH_2-NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 17 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1993:604650 HCAPLUS

DOCUMENT NUMBER:

INVENTOR (S):

119:204650

TITLE:

Compatible thermoplastic blends with low discoloration Hotsuta, Hiroshi; Kitazawa, Naoki; Suqita, Yasuhisa;

Oota, Katsuhisa

PATENT ASSIGNEE(S):

Idemitsu Petrochemical Co, Japan; Dai Ichi Kogyo

Seiyaku Co Ltd

SOURCE:

Jpn. Kokai Tokkyo Koho, 35 pp.

CODEN: JKXXAF

DOCUMENT TYPE:

Patent Japanese

LANGUAGE:

NT: 1

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. -------------------------JP 05032902 A2 19930209 JP 1991-191632 19910731 <--PRIORITY APPLN. INFO.: JP 1991-191632

The title blends with good impact resistance comprise (A) 5-95% thermoplastic polymers bearing groups reactive to amines, (B) 95-5% olefin and/or styrene polymers, and (C) 0.05-20 phr (of A+B) compatibilizers bearing units derived from vinyl compds., maleic acids modified with diamines and formyl-forming compds., etc. Thus, heating a maleated polypropylene with an ethylenediamine p-toluenesulfonate salt at reflux in xylene and DMF and detosylating gave a product bearing amine, formamide and imide groups. A blend containing the above product 2, a polycarbonate 90, and a polypropylene 10 parts gave test pieces without phase separation and good impact strength.

IT7294-10-2DP, reaction products with maleated vinyl polymers,

modified to bear formamide groups

RL: PREP (Preparation)

(compatibilizing agents for thermoplastic blends, manufacture of)

RN 7294-10-2 HCAPLUS

CN 1,2-Ethanediamine, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 107-15-3 CMF C2 H8 N2

 $H_2N-CH_2-CH_2-NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

HO3S

L37 ANSWER 18 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:540018 HCAPLUS

DOCUMENT NUMBER: 119:140018

TITLE: Formamide group-containing copolymer, its preparation,

> and thermoplastic compositions containing it. Kitazawa, Naoki; Hotta, Hiroshi; Sumi, Hideyuki;

INVENTOR(S): Kikuta, Manabu; Sugita, Yasuhisa; Ohta, Katsutoshi

Daiichi Koqyo Seiyaku Co., Ltd., Japan PATENT ASSIGNEE(S): SOURCE:

Eur. Pat. Appl., 90 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent English LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 525793	A1	19930203	EP 1992-113094	19920731 <
EP 525793	B1	19960522		
R: BE, CH, DE,	FR, GB	, LI, NL		
JP 05032715	A2	19930209	JP 1991-191595	19910731 <
JP 3048425	B2	20000605		
JP 05032716	A2	19930209	JP 1991-191596	19910731 <
JP 3048426	B2	20000605		
US 5420210	Α	19950530	US 1992-921343	19920729 <
US 5373065	Α	19941213	US 1993-149525	19931109 <
PRIORITY APPLN. INFO.:			JP 1991-191595 A	19910731
			JP 1991-191596 A	19910731
			US 1992-921343 A	3 19920729

The copolymer is prepared by reacting a polymer with recurring units from AB styrene, olefin (derivs.), dienes, acid anhydrides (such as maleic anhydride) with a salt of a primary diamine in presence of a formyl group-containing compound (e.g., formamide) to effect imidation or amidation, and deacidifying with base. Thus, a 95:5 (molar) styrene-maleic anhydride copolymer in xylene was added dropwise to a DMF solution of ethylenediamine p-toluenesulfonate at 80-140° with azeotropic distillation to remove H2O, and precipitation in MeOH gave a polymer (I) with formamide and primary NH2

at 89:11 molar ratio, resp. Blending Tuflon A 200 polycarbonate 5, Polypro E 100G polypropylene 95, and I 5 parts, kneading, and injection molding gave white test pieces showing impact strength (23°; JIS-K

14034-59-4P, Ethylenediamine p-toluenesulfonate IT

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction of, with maleic anhydride copolymers)

RN14034-59-4 HCAPLUS

1,2-Ethanediamine, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME) CN

CM 1

CRN 107-15-3 CMF C2 H8 N2

 $H_2N-CH_2-CH_2-NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 19 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER:

DOCUMENT NUMBER:

1993:450177 HCAPLUS

119:50177

TITLE: Amino group-containing polymers and manufacture

thereof

Hotta, Hiroshi; Kitazawa, Naoki; Sumi, Hideyuki INVENTOR(S):

PATENT ASSIGNEE(S): Daiichi Kogyo Seiyaku Co., Ltd., Japan

Jpn. Kokai Tokkyo Koho, 11 pp. SOURCE:

CODEN: JKXXAF

DOCUMENT TYPE: Patent Japanese LANGUAGE:

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04296309	A2	19921020	JP 1991-85736	19910327 <
JP 3068233	B2	20000724		
PRIORITY APPLN. INFO.:			JP 1991-85736	19910327
GI				

The title polymers, useful as reagents, adhesives, polymer AB compatibilizers, etc., comprise 40-99.8 mol % units CH2CR1R2 (R1-2 = H, alkyl, cycloalkyl, aryl, alkenyl, alkoxy, halo, etc.), 0-50 mol % units CR3:CR4 (R3-4 = H, alkyl, alkenyl, halo), and 0.2-60 mol % units I (R5-6 = H, alkyl, aryl; R7 = alkylene, cycloalkylene, arylene, arylalkylene, polyoxyalkylene) and are prepared by treating maleic anhydride copolymers with a diamine salt followed by treatment with a base for acid removal. A 95:5 styrene-maleic anhydride copolymer was treated with ethylenediamine p-toluenesulfonate followed by K2CO3 in aqueous MeOH to give a polymer containing

imide groups and forming a 10% xylene solution showing viscosity 680 cP. IT 14034-59-4DP, Ethylenediamine p-toluenesulfonate, imidation

products with maleic anhydride copolymers RL: PREP (Preparation)

(preparation of)

RN14034-59-4 HCAPLUS

1,2-Ethanediamine, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME) CN

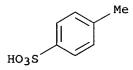
CM1

CRN 107-15-3 CMF C2 H8 N2

H2N-CH2-CH2-NH2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S



L37 ANSWER 20 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1993:450176 HCAPLUS

DOCUMENT NUMBER: 119:50176

TITLE: Amino group-containing polymers and manufacture

thereof

INVENTOR(S): Hotta, Hiroshi; Kitazawa, Naoki; Sumi, Hideyuki

PATENT ASSIGNEE(S): Daiichi Kogyo Seiyaku Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 04296308	A2	19921020	JP 1991-85735	19910327 <
JP 3068232	B2	20000724		
PRIORITY APPLN. INFO.:			JP 1991-85735	19910327
GI				

The title polymers useful as polymeric amine reagents, functional polymer starting materials, adhesives, polymer compatibilizers, etc. comprise 20-99.8 mol% -CH2C(R1)(R2) - unit, 0-50 mol% -C(R3):C(R4) - unit, and 0.2-30 mol% I unit (R1, R2, R5, R6, R7 = H, alkyl, cycloalkyl, aryl, alkenyl, alkoxy, alkoxycarbonyl, alkylcarboxy, alkylcarbonyl, arylcarbonyl, halogen, nitrile group; R3, R4 = H, alkyl, alkenyl, halogen; R8 = direct bond, methylene, ethylene; R9, R10 = H, alkyl, aryl; R11 = alkylene, cycloalkylene, arylene, arylalkylene, polyoxyalkylene; R12 = H, alkyl; n = 1-10) and are prepared by treating copolymers containing maleic anhydride derivs. in place of I units, with a diamine salt, followed by treatment with a base for acid removal. A maleated polypropylene was treated with ethylenediamine p-toluenesulfonate then with K carbonate in water-methanol mixture to give an imidized polymer with 10% Tetralin solution viscosity 165 cP at 25°.

IT 14034-59-4DP, Ethylenediamine p-toluenesulfonate, reaction
products with maleated polyolefins
RL: PREP (Preparation)

(preparation of)

RN 14034-59-4 HCAPLUS

CN 1,2-Ethanediamine, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 107-15-3 CMF C2 H8 N2

 $H_2N-CH_2-CH_2-NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

HO3S Me

L37 ANSWER 21 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:482365 HCAPLUS

DOCUMENT NUMBER: 117:82365

TITLE: Synthesis, spectroscopic and x-ray structural

characterization of cadmium complex [Cd(linpen)]2+, a model for metal complexes of the chelating polymer

polyethyleneimine (linpen = linear

pentaethylenehexamine)

AUTHOR(S): Strasdeit, Henry

CORPORATE SOURCE: Fachbereich Chem., Univ. Oldenburg, Oldenburg,

D-W-2900, Germany

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences

**(1992)**, 47(6), 829-36

CODEN: ZNBSEN; ISSN: 0932-0776

DOCUMENT TYPE: Journal LANGUAGE: English

The isolation of 3,6,9,12-tetraazatetradecane-1,14-diamine (linear isomer of pentaethylenehexamine, linpen) from a tech. polyamine mixture is described. In MeOH, linpen acts as a hexadentate ligand towards [Cd(linpen)](BPh4)2 (1), [Cd(linpen)](BPh4)2.2DMSO (2), and cadmium(II). [Cd(linpen)] (BF4)2 (3) were isolated and characterized by elemental anal., spectroscopy and x-ray powder diffraction. The 113Cd NMR resonance of 1 is at 351 ppm (0.30 M in DMSO-d6, standard: 0.10 M Cd(ClO4)2 in D2O). 2 And 3 were structurally characterized by single-crystal x-ray diffraction. Both compds. contain discrete [Cd(linpen)]2+ complexes. The hexamine wraps around the metal ion in a helical manner. This results in a strong distortion of the coordination polyhedron. The mean Cd-N bond lengths are 2.38 Å and 2.37 Å for 2 and 3, resp. Models for MN6 centers in metal-polyethyleneimine (PEI) complexes are derived from the structure of [Cd(linpen)]2+. For example, loops at the MN6 site in mols. of linear polyethyleneimine are proposed.

IT 98405-89-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation in isolation of linear from tech. pentaethylenehexamine and detosylation of, by sodium methoxide)

98405-89-1 HCAPLUS RN

3,6,9,12-Tetraazatetradecane-1,14-diamine, hexakis(4-CN methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 4067-16-7 CMF C10 H28 N6

PAGE 1-A

H<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-

PAGE 1-B

— cн<sub>2</sub>- ин<sub>2</sub>

CM

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 22 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:552411 HCAPLUS

DOCUMENT NUMBER: 113:152411

TITLE: Preparation of 2,3-dihydro-2-(4,5-dihydroimidazol-2-

yl) indoles as  $\alpha$ 2-adrenergic antagonists and as

antiglaucoma agents

INVENTOR(S): Huebner, Charles F.; Francis, John E.

PATENT ASSIGNEE(S): Ciba-Geigy Corp., USA

SOURCE: U.S., 6 pp. Division of U.S. Ser. No. 771,935.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.		DATE	
US 4908376	Α	19900313	US 1987-15820		19870217	<
US 4912125	A	19900327	US 1985-771935		19850903	<
PRIORITY APPLN. INFO.:			US 1985-771935	<b>A3</b>	19850903	
OTHER SOURCE(S):	CASRE	ACT 113:15241	11: MARPAT 113:152411			

GI

AB The title compds. [I; R = alkyl, alkoxy, halo, CF3; R1 = H, alkyl, alkoxycarbonyl, (un)substituted Ph, phenylalkyl; R2 = R3 = H or R2 = H and R3 = alkyl] were prepared as α2-adrenergic antagonists and antiglaucoma agents (no data). PhCH2NPhNH2 was cyclocondensed with MeCOCO2Et and the product treated with CF3CO2H and NaBH4 to give Et 1-benzyl-2,3-dihydroindole-2-carboxylate which was added to (H2NCH2)2 which had reacted with Me3Al in PhMe and the whole refluxed 3 h to give title compound II.

IT 7294-10-2P, Ethylenediamine tosylate

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of adrenergic antagonists and antiglaucoma agents)

RN 7294-10-2 HCAPLUS

CN 1,2-Ethanediamine, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 107-15-3 CMF C2 H8 N2

 $H_2N-CH_2-CH_2-NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 23 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:551764 HCAPLUS

DOCUMENT NUMBER: 113:151764

TITLE: An expedient synthesis of vicinal diamines from

alkenes and cycloalkenes

AUTHOR(S): Osowska-Pacewicka, Krystyna; Zwierzak, Andrzej

CORPORATE SOURCE: Inst. Org. Chem., Tech. Univ., Lodz, PL-90-924, Pol.

SOURCE:

Synthesis (1990), (6), 505-8

CODEN: SYNTBF; ISSN: 0039-7881

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 113:151764

RCHBrCHR1NHP(0)(OEt)2 [I; R = H, R1 = Pr, Bu, Ph; R = Me, R1 = Ph; RR1 = Me2, (CH2)4, o-CH2C6H4] were converted to H2NCHRCHR1NH2.2 p-MeC6H4SO3H by successive reaction with NaN3, Staudinger reaction with P(OEt)3, and

hydrolysis with aqueous p-MeC6H4SO3H. Reaction of I [RR1 = (CH2)4, o-CH2C6H4] proceeded stereospecifically to give the cis-diamines. Stereochem.

control was also obtained in the azidation of BrCHMeCHMeBr.

IT 129687-42-9P 129687-43-0P 129687-45-2P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN129687-42-9 HCAPLUS

CN 1,2-Pentanediamine, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM

CRN 52940-41-7 CMF C5 H14 N2

$$\begin{array}{c} & ^{\rm NH_2}\\ |\\ {\rm H_2N-CH_2-CH-Pr-n} \end{array}$$

CM

CRN 104-15-4 CMF C7 H8 O3 S

RN 129687-43-0 HCAPLUS

CN 1,2-Hexanediamine, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 13880-27-8 CMF C6 H16 N2

$$^{\rm NH_2}_{\rm H_2N-CH_2-CH-Bu-n}$$

CM

CRN 104-15-4

CMF C7 H8 O3 S

RN 129687-45-2 HCAPLUS

CN 1,2-Ethanediamine, 1-phenyl-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 5700-56-1 CMF C8 H12 N2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 24 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1988:131774 HCAPLUS

DOCUMENT NUMBER: 108:131774

TITLE: A novel very strong basic pentacyclic "proton sponge"

with vinamidine structure

AUTHOR(S): Schwesinger, Reinhard; Missfeldt, Michael; Peters,

Karl; Georg von Schnering, Hans

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Freiburg, Freiburg,

D-7800, Fed. Rep. Ger.

SOURCE: Angewandte Chemie (1987), 99(11), 1210-12

CODEN: ANCEAD; ISSN: 0044-8249

DOCUMENT TYPE: Journal LANGUAGE: German

OTHER SOURCE(S): CASREACT 108:131774

GI

AB The title compds. I [R = H (II), Me] and III were prepared and their high kinetic basicity and nucleophilicity observed. The conformations of II·HBPh4 and II·2HClO4 were crystallog. determined and the nature of the intramol. H-bonding discussed. The effects of proximate nitrogen atom lone electron pairs on the basicity and nucleophilicity were also discussed.

IT 111161-09-2P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and conversion to pentacyclic vinamidine analog) 111161-09-2 HCAPLUS

CN Propanedinitrile, [1-[2-[[2-[[2-[(2-aminoethyl)amino]ethyl]amino]ethyl]amino]ethyl]-2-imidazolidinylidene]-, tetrakis(4-methylbenzenesulfonate)
(9CI) (CA INDEX NAME)

CM 1

RN

CRN 111161-08-1 CMF C14 H26 N8

$$\begin{array}{c|c} & CN & \\ & C-CN & \\ &$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 25 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1988:75804 HCAPLUS

DOCUMENT NUMBER:

108:75804

TITLE:

Specific adsorbents for peptide antibiotic-

synthesizing enzyme system Gramicidin S synthetase. 1.

Preparation of low molecular weight spacer/ligand

compounds

AUTHOR(S):

Schluensen, Juergen; Manecke, Georg

CORPORATE SOURCE:

Inst. Org. Chem., Freie Univ. Berlin, Berlin,

D-1000/13, Fed. Rep. Ger.

SOURCE:

Makromolekulare Chemie (1987), 188(12),

3005-16

CODEN: MACEAK; ISSN: 0025-116X

DOCUMENT TYPE:

Journal

LANGUAGE:

German

AB Several amide derivs. of phenylalanine and proline were prepared as spacer-ligand compds. by reaction of unprotected or monoprotected aliphatic and aromatic diamines and monoamines with the succinimido esters of the N-protected amino acids. The formation of diacylated aliphatic diamines was fast under normal conditions. In the case of aromatic diamines, the presence of a base is necessary. For the preparation of monoacylated diamines, best results were obtained with monoprotected diamines. The acylated diamines were purified by column chromatog. or by extraction

112670-22-1P 112670-29-8P IT

> RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of)

RN 112670-22-1 HCAPLUS

CN Benzenesulfenamide, N-(2-aminoethyl)-2-nitro-, mono(4-

methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 112670-21-0 CMF C8 H11 N3 O2 S

CM 2

104-15-4 CRN CMF C7 H8 O3 S

112670-29-8 HCAPLUS RN

Carbamic acid, (2-aminoethyl)-, 1,1-dimethylethyl ester, CN mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1 CRN 57260-73-8 CMF C7 H16 N2 O2

$$\begin{array}{c} \text{O} \\ || \\ \text{t-BuO- C- NH- CH}_2\text{-- CH}_2\text{-- NH}_2 \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 26 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:32841 HCAPLUS

DOCUMENT NUMBER: 106:32841

TITLE: Dihydropyridine-3,5-dicarboxylates incorporating

aryloxypropanolamine moieties

INVENTOR(S): Poindexter, Graham S.

PATENT ASSIGNEE(S): Bristol-Myers Co., USA
SOURCE: PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

TENT NO.			KIND	DATE	APPLICATION NO.		DATE
			A1	19860509	WO 1985-US2088		19851025 <
W: JP							
RW: AT,	BE,	CH,	DE, FR	, GB, IT,	LU, NL, SE		
4994476			Α	19910219	US 1985-779188		19850923 <
201558			A1	19861120	EP 1985-905684		19851025 <
R: AT,	BE,	CH,	DE, FR	, GB, IT,	LI, LU, NL, SE		
62501004			T2	19870423	JP 1985-505014		19851025 <
Y APPLN.	INFO.	:			US 1984-666848	Α	19841031
					US 1985-779188	A	19850923
					WO 1985-US2088	W	19851025
	4994476 201558 R: AT, 62501004	8602640 W: JP RW: AT, BE, 4994476 201558 R: AT, BE, 62501004	8602640 W: JP RW: AT, BE, CH, 4994476 201558 R: AT, BE, CH,	8602640 A1 W: JP RW: AT, BE, CH, DE, FR 4994476 A 201558 A1 R: AT, BE, CH, DE, FR 62501004 T2	8602640 A1 19860509 W: JP RW: AT, BE, CH, DE, FR, GB, IT, 4994476 A 19910219 201558 A1 19861120 R: AT, BE, CH, DE, FR, GB, IT, 62501004 T2 19870423	8602640 A1 19860509 WO 1985-US2088 W: JP RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE 4994476 A 19910219 US 1985-779188 201558 A1 19861120 EP 1985-905684 R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE 62501004 T2 19870423 JP 1985-505014 Y APPLN. INFO.: US 1984-666848 US 1985-779188	8602640 A1 19860509 WO 1985-US2088 W: JP RW: AT, BE, CH, DE, FR, GB, IT, LU, NL, SE 4994476 A 19910219 US 1985-779188 201558 A1 19861120 EP 1985-905684 R: AT, BE, CH, DE, FR, GB, IT, LI, LU, NL, SE 62501004 T2 19870423 JP 1985-505014 Y APPLN. INFO.: US 1984-666848 A US 1985-779188 A

GI

$$R^{2}O_{2}C$$
 $CO_{2}XR^{1}$ 
 $R^{4}$ 
 $R^{4}$ 

AB Title compds. I [R1 = NHCH2CH(OH)CH2OR5, X1OCH2CH(OH)CH2NR6R7; R2, R3 = alkyl, hydroxyalkyl, alkoxyalkyl, aminoalkyl; R4 = alkyl, hydroxyalkyl, alkoxyalkyl, aminoalkyl, Ph, thienyl; R5 = (substituted) Ph, naphthyl, 4-(4-morpholino)-1,2,5-thiadiazol-3-yl; R6, R7 = H, alkyl; X = bond, (substituted) alkylene, optionally interrupted by O, N, CON, NC(S)N; X1 = (substituted) naphthyldiyl, phenylene] are prepared These compds. are useful for treatment of cardiovascular disorders, as they are both β-blockers and Ca antagonists (no data); the β-blocker is incorporated as R1. Thus, 3-O2NC6H4CH:CAcCO2Me (II) was prepared from 3-O2NC6H4CHO and Me acetylacetonate, and C1(CH2)3O2CCH2CO2Me (III) was prepared from diketene and C1(CH2)3OH. II reacted with III to give pyridinedicarboxylate IV, which condensed with 2-MeC6H4OCH2CH(OH)CH2NH2 to form pyridinedicarboxylate V, which incorporates the β-blocking moiety.

V

### IT 105461-05-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of, as calcium-β-blocker)

RN 105461-05-0 HCAPLUS

CN 3-Pyridinecarboxylic acid, 5-[[(2-aminoethyl)amino]carbonyl]-1,4-dihydro-2,6-dimethyl-4-(3-nitrophenyl)-, methyl ester, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 105460-47-7 CMF C18 H22 N4 O5

$$\begin{array}{c|c} & \text{NO}_2 \\ & \text{O} \\ & \text{II} \\ & \text{MeO-C} \\ & \text{Me} \\ & \text{Me} \end{array} \begin{array}{c} \text{NO}_2 \\ & \text{C-NH-CH}_2\text{-CH}_2\text{-NH}_2 \\ & \text{Me} \\ & \text{Me} \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 27 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:169021 HCAPLUS

DOCUMENT NUMBER: 104:169021

TITLE: Polyethylenepolyamines

INVENTOR(S): Araki, Nagao; Kubo, Takao; Kawamura, Shigeyuki

PATENT ASSIGNEE(S): Nippon Kayaku Co., Ltd., Japan SOURCE: Jpn. Kokai Tokkyo Koho, 6 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA	ATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JF	60188351	A2	19850925	JP 1984-42830	19840308 <
PRIORIT	TY APPLN. INFO.:			JP 1984-42830	19840308
				ful as electrolytic car:	
pr	repared by hydrolys	sis of t	the sorrespon	nding arenesulfonamides	. Thus,

prepared by hydrolysis of the sorresponding arenesulfonamides. Thus, heptaethyleneoctamine octatosyl derivative, prepared in 5 steps from triethylenetetramine, was stirred in 90% H2SO4 at 100° for 3 h to give 85% heptaethyleneoctamine.

IT 101613-40-5P 101613-41-6P

RN 101613-40-5 HCAPLUS

CN Benzenesulfonic acid, 4-methyl-, octaamide with 3,6,9,12,15,18,21,24-octaazahexacosane-1,26-diamine (9CI) (CA INDEX NAME)

CM 1

CRN 5763-77-9 CMF C18 H48 N10

PAGE 1-A

H2N-CH2-CH2-NH-CH2-CH2-NH-CH2-CH2-NH-CH2-CH2-NH-CH2-

PAGE 1-B

-- CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH<sub>2</sub>

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 101613-41-6 HCAPLUS

CN Benzenesulfonic acid, 4-methyl-, hexaamide with 3,6,9,12,15,18-hexaazaeicosane-1,20-diamine (9CI) (CA INDEX NAME)

CM 1

CRN 4617-43-0 CMF C14 H38 N8

PAGE 1-A

H<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-

PAGE 1-B

 $-CH_2-NH-CH_2-CH_2-NH-CH_2-CH_2-NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 28 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1985:541408 HCAPLUS

DOCUMENT NUMBER:

103:141408

TITLE:

A simple method of polyamine purification

AUTHOR (S):

Stapleton, Ian W.

CORPORATE SOURCE:

Div. Protein Chem., CSIRO, Parkville, 3052, Australia

SOURCE:

Australian Journal of Chemistry (1985),

38(4), 633-6 CODEN: AJCHAS; ISSN: 0004-9425

DOCUMENT TYPE:

Journal

LANGUAGE:

English

OTHER SOURCE(S):

CASREACT 103:141408

A simple procedure for the large-scale purification of com. polyethyleneamines

[H2N(CH2CH2NH)nH; n = 2-5) is described in which the pertosylate salt

separates as a crystalline solid from aqueous solution The salts require no

further

purification except for pentaethylenehexamine (n = 5), which requires recrystn. from water. The free bases are regenerated from the tosylate salt by an

anion-exchange resin.

IT 98405-86-8P 98405-87-9P 98405-88-0P

98405-89-1P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation, IR, and recovery of amine from)

98405-86-8 HCAPLUS RN

1,2-Ethanediamine, N-(2-aminoethyl)-, tris(4-methylbenzenesulfonate) (9CI) CN

(CA INDEX NAME)

CM

CRN 111-40-0

CMF C4 H13 N3

 $H_2N-CH_2-CH_2-NH-CH_2-CH_2-NH_2$ 

CM

CRN 104-15-4

CMF C7 H8 O3 S

RN 98405-87-9 HCAPLUS CN 1,2-Ethanediamine, N,N'-bis(2-aminoethyl)-, tetrakis(4methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 112-24-3 CMF C6 H18 N4

 $_{\rm H_2N^-\,CH_2^-\,CH_2^-\,NH^-\,CH_2^-\,CH_2^-\,NH^-\,CH_2^-\,CH_2^-\,NH_2}$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 98405-88-0 HCAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-N'-[2-[(2-aminoethyl)amino]ethyl]-, pentakis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 112-57-2 CMF C8 H23 N5

 $H_2N-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2-CH_2-NH-CH_2-CH_2-NH_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 98405-89-1 HCAPLUS

CN 3,6,9,12-Tetraazatetradecane-1,14-diamine, hexakis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 4067-16-7

CMF C10 H28 N6

PAGE 1-A

H<sub>2</sub>N-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-CH<sub>2</sub>-NH-CH<sub>2</sub>-

PAGE 1-B

 $- ch_2 - nh_2$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 29 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1983:575760 HCAPLUS

DOCUMENT NUMBER: 99:175760

TITLE: 2-(2-Alkoxyethyl)-2-imidazolines.

INVENTOR(S): Jianu, Ionel Vasile; Maurer, Ewald Vilian PATENT ASSIGNEE(S): Intreprinderea de Detergenti, Timisoara, Rom.

SOURCE: Rom., 5 pp.

CODEN: RUXXA3

DOCUMENT TYPE: Patent LANGUAGE: Romanian

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
RO 77367	В	19810817	RO 1979-97311	19790420 <
PRIORITY APPLN. INFO.:			RO 1979-97311 A	19790420
GI				

$$RO(CH_2CH_2O)_nCH_2CH_2 \frac{1}{n} N(CH_2CH_2NH)_mH$$

AB Title compds. I (n = 0, 1, 2, 3, 4; m = 0, 1, 2; R = alkyl), useful as antistatic agents for textiles (no data), were prepared from the resp. RO(CH2CH2O)nCH2CH2CN and H2NCH2CH2NH(CH2CH2NH)mH. Thus, BuCHEtCH2OCH2CH was heated with ethylenediamine tosylate at 250° and the mixture was treated with NaOH to give I (n = m = 0, R = BuCHEtCH2).

Ι

IT 87470-27-7P 87470-31-3P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 87470-27-7 HCAPLUS

CN 1,2-Ethanediamine, N,N'-bis(2-aminoethyl)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 112-24-3 CMF C6 H18 N4

 $_{\rm H_2N^-\,CH_2^-\,CH_2^-\,NH^-\,CH_2^-\,CH_2^-\,NH^-\,CH_2^-\,CH_2^-\,NH_2}$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 87470-31-3 HCAPLUS

CN 1,2-Ethanediamine, N-(2-aminoethyl)-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 111-40-0 CMF C4 H13 N3

H2N-CH2-CH2-NH-CH2-CH2-NH2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 30 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN ACCESSION NUMBER: 1982:16552 HCAPLUS

DOCUMENT NUMBER:

96:16552

TITLE:

The synthesis of new polymer derivatives of ATP by radical copolymerization and their coenzymic activity

AUTHOR(S):

Yamazaki, Yoshimitsu; Maeda, Hidekatsu

CORPORATE SOURCE:

Agency Ind. Sci. Technol., Minist. Int. Trade Ind.,

Ibaraki, 305, Japan

SOURCE:

Agricultural and Biological Chemistry (1981

), 45(9), 2091-103

CODEN: ABCHA6; ISSN: 0002-1369

DOCUMENT TYPE:

Journal

LANGUAGE:

English

Three polymerizable ATP derivs., N6-[N-(6-methacrylamidohexyl)carbamoylmet hyl]-, N6-[N-[2-[N-(2-methacrylamidoethyl)carbamoyl]ethyl]carbamoylmethyl]-, and N6-[N-[N-(2-hydroxy-3-methacrylamidopropyl)carbamoylmethyl]carbamoyl methyl]-ATP, were synthesized and radical-copolymd. with comonomers [acrylamide, N-(2-hydroxyethyl)-, N-ethyl-, N,N-diethylacrylamide, acrylic acid, and 6-methacrylamidohexylammonium chloride) to obtain 18 new polymer derivs. of ATP. The mol. weight distributions were controlled by appropriate initiator concns. The monomeric and polymeric ATP derivs. were all phosphate donors in both the hexokinase and glycerol kinase reactions. Parameters of the observed coenzymic activities (Km and Vmax) are discussed in relation to the structures of the derivs.

TТ 80224-30-2P

> RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with methacrylic acid)

80224-30-2 HCAPLUS

Propanamide, N-(2-aminoethyl)-3-[(triphenylmethyl)amino]-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM

CRN 80224-29-9 CMF C24 H27 N3 O

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 31 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1981:532502 HCAPLUS

DOCUMENT NUMBER:

TITLE: Biphenylmethane derivative and pharmaceutical

compositions containing it

INVENTOR(S): Klemm, Kurt; Haerlin, Ruediger; Zick, Franz; Baron,

Lothar; Pruesse, Wolfgang; Krueger, Uwe

PATENT ASSIGNEE(S): Byk-Gulden Lomberg Chemische Fabrik G.m.b.H., Fed.

Rep. Ger.

SOURCE: Eur. Pat. Appl., 34 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE				
EP 29990	A1	19810610	EP 1980-107328	19801125 <				
EP 29990	B1	19820908						
R: AT, BE, CH,	DE, FR	, GB, IT, LU	, NL, SE					
AT 1523	E	19820915	AT 1980-107328	19801125 <				
IL 61600	A1	19840629	IL 1980-61600	19801201 <				
AU 8064997	A1	19810611	AU 1980-64997	19801202 <				
AU 535714	B2	19840405						
DK 8005175	Α	19810605	DK 1980-5175	19801203 <				
ZA 8007544	Α	19811125	ZA 1980-7544	19801203 <				
ES 497410	A1	19820101	ES 1980-497410	19801203 <				
JP 56113754	A2	19810907	JP 1980-171453	19801204 <				
PRIORITY APPLN. INFO.:			CH 1979-10763	A 19791204				
			EP 1980-107328	A 19801125				

GI

AB I and a number (.apprx.10) of its salts (e.g., Ba, piperazine, dimethylpiperazine) were prepared by condensation of 4,2-Me(HO)C6H3SO3H (or the appropriate salt of it) with HCHO, or by treatment of I with the appropriate base.

IT 79093-75-7P 79093-88-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 79093-75-7 HCAPLUS

CN Benzenesulfonic acid, 3,3'-methylenebis[6-hydroxy-4-methyl-, compd. with 1,2-ethanediamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 78480-14-5 CMF C15 H16 O8 S2

HO 
$$CH_2$$
  $CH_2$   $SO_3H$ 

CM 2

CRN 107-15-3 CMF C2 H8 N2

 $H_2N-CH_2-CH_2-NH_2$ 

RN 79093-88-2 HCAPLUS

CN Benzenesulfonic acid, 2-hydroxy-4-methyl-, compd. with 1,2-ethanediamine (2:1) (9CI) (CA INDEX NAME)

CM 1

CRN 22356-80-5 CMF C7 H8 O4 S

CM 2

CRN 107-15-3 CMF C2 H8 N2

 $H_2N-CH_2-CH_2-NH_2$ 

L37 ANSWER 32 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1978:508501 HCAPLUS

DOCUMENT NUMBER:

89:108501

TITLE:

Synthesis of compounds with potential antitubercular

activity in the group of hydrazinoamines. XIV. Reactions of 2-aminoethylhydrazine with ketones

AUTHOR (S):

Ropenga, Jacek; Grudzinski, Stefan

CORPORATE SOURCE:

Inst. Technol. Chem. Pharm. Prod., Sch. Med., Lodz,

Pol.

SOURCE:

Acta Poloniae Pharmaceutica (1977), 34(4),

391-7

CODEN: APPHAX; ISSN: 0001-6837

DOCUMENT TYPE:

Journal

LANGUAGE:

Polish

OTHER SOURCE(S):

CASREACT 89:108501

Refluxing H2NCH2CH2NHNH2 (I) 1 h with an aliphatic ketone gave

H2NCH2CH2NHN:CRR1 (II; R = Me, R1 = Me, Et, Pr); salts of I were also

prepared Treating II (R = R1 = Me) with 4-02NC6H4CHO gave

4-02NC6H4CH:NCH2CH2NHN:CMe2. Me2C:NCH2CH2NHN:CMe2 was prepared by heating I with Me2CO for 9 h. Treating I with PhCOMe gave a mixture of the mono- and bis(1-phenylethylidene) derivs.

IT 67232-86-4P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as potential antitubercular substances)

RN67232-86-4 HCAPLUS

CN 2-Propanone, (2-aminoethyl) hydrazone, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM

67232-85-3 CRN

CMF C5 H13 N3

 $Me_2C = N - NH - CH_2 - CH_2 - NH_2$ 

CM 2

104-15-4 CRN CMF C7 H8 O3 S

L37 ANSWER 33 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1977:170767 HCAPLUS

DOCUMENT NUMBER:

86:170767

TITLE:

Synthesis of 1,2-diaminopropane derivatives. I. Preparation of D,L-1-dimethylamino-2-aminopropane

AUTHOR (S):

Grudzinski, Stefan; Gronek, Maria; Zalega, Urszula

CORPORATE SOURCE:

Inst. Technol. Chem. Pharm. Prod., Sch. Med., Lodz,

Pol.

SOURCE:

Acta Poloniae Pharmaceutica (1976), 33(5),

571-6

CODEN: APPHAX; ISSN: 0001-6837

DOCUMENT TYPE:

Journal

LANGUAGE:

Polish

MeCH(NH2)CH2NMe2 (I) was prepared in 49% yield by hydrogenation (Raney Ni) of DL-MeCH(NO2) CH2NMe2 (II) in MeOH; the yield was increased to 78.5% when I was isolated from the reaction mixture as the 3,5-dinitrobenzoate. acetylated to give 48% yield of the acetyl derivative II was prepared from DL-MeCH(NO2)CH2OH and aqueous Me2NH.

IT 62689-57-0P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of)

RN 62689-57-0 HCAPLUS

CN 1,2-Propanediamine, N1,N1-dimethyl-, bis(4-methylbenzenesulfonate) (9CI)

(CA INDEX NAME)

CM 1

CRN 108-15-6 CMF C5 H14 N2

 $\begin{array}{c} \mathrm{NH_2} \\ | \\ \mathrm{Me-CH-CH_2-NMe_2} \end{array}$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 34 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1976:592321 HCAPLUS

DOCUMENT NUMBER:

85:192321

TITLE:

Synthesis of compounds from the hydrazinoamine group

with expected antitubercular activity. XII. Condensation of 2-aminoethylhydrazine with p- and

m-nitrobenzaldehydes

AUTHOR(S): Grudzinski, Stefan; Strumillo, Jozef

CORPORATE SOURCE: Inst. Technol. Chem. Pharm. Prod., Sch. Med., Lodz,

Pol.

SOURCE:

Acta Poloniae Pharmaceutica (1976), 33(1),

31-8

CODEN: APPHAX; ISSN: 0001-6837

DOCUMENT TYPE:

Journal

LANGUAGE:

Polish

OTHER SOURCE(S):

CASREACT 85:192321

AB 4-O2NC6H4CH:NNH(CH2)2NHR (I; R = H) was prepared in 90% yield by treating H2NNH(CH2)2NH2 (II) in refluxing MeOH with 4-O2NC6H4CHO. Treating II with cyanomethyl hippurate or 4-nitrobenzoate gave I (R = COCH2NHCOPh, COC6H4NO2-4, resp.). Several salts of II and the analogous products from

3-02C6H4CHO were also prepared

IT 61146-09-6P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 61146-09-6 HCAPLUS

CN Benzaldehyde, 4-nitro-, (2-aminoethyl)hydrazone, 4-methylbenzenesulfonate

(9CI) (CA INDEX NAME)

CM 1

CRN 36780-83-3 CMF C9 H12 N4 O2

CM

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 35 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

2

ACCESSION NUMBER: 1976:462634 HCAPLUS

DOCUMENT NUMBER: 85:62634

TITLE: Amino alcohols INVENTOR(S): Gipson, Robert M.

PATENT ASSIGNEE(S): USA

SOURCE: U.S., 8 pp. Division of U.S. 3,872,116.

CODEN: USXXAM

DOCUMENT TYPE: Patent

LANGUAGE: English

FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE -----\_ \_ \_ \_ ---------------US 3954873 Α 19760504 US 1974-461549 19740417 <--US 3872116 Α 19750318 US 1972-263552 19720616 <--CA 1006520 Α1 19770308 CA 1973-170548 19730507 <--GB 1440112 Α 19760623 GB 1973-27412 19730608 <--BE 800944 **A1** 19731217 BE 1973-1005157 19730615 <--NL 7308403 Α 19731218 NL 1973-8403 19730615 <--JP 49061108 A2 19740613 JP 1973-67649 19730615 <--FR 2213270 **A1** 19740802 FR 1973-21938 19730615 <--PRIORITY APPLN. INFO.: US 1972-263552 A3 19720616 GI

AB Ethanolamines, e.g., HOCRR1CH2NR2R3 [I; R = C6H13, R1 = C10H21; R = R1 = C8H17; R = C6H13, R1 = C8H17; R = C4H9, R1 = C6H13; R = C8H17, R1 = C10H21; R = C12H25, R1 = C10H21; R2 = R3 = Me, CH2CH2OH; NR2R3 = morpholino; R2 = H, R3 = CH2CH2NH2, CH2CH2NHCH2CH2NH2, (CH2)3NH(CH2)2NH2] were prepared by reaction of epoxides II with R2NHR3. Thus, reaction of morpholine, HCl, II (R = R1 = C8H17), and II (R = C6H13, R1 = C10H21) at 128-30° for 20 hr gave I (R = C6H13, R1 = C10H21, R2R3N = morpholino) and I (R = R1 = C8H17, R2R3N = morpholino). I (R, R1 = alkyl; R2R3N = morpholino; R2,R3 = H, alkyl) oleates, acetates and p-toluenesulfonates were effective. Five HOCRR1CH2N+R2R3R4 X- (e.g., R = decyl, R1 = octyl, R2 = R3 = Me, R4 = benzyl, X = C1) were prepared and were tested for their surface active properties (e.g., foaming power and herbicidal activity).

IT 59941-43-4P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and use as corrosion inhibitors)

RN 59941-43-4 HCAPLUS

CN Heneicosanol, [[(2-aminoethyl)amino]methyl]-, 4-methylbenzenesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 59941-42-3 CMF C24 H52 N2 O CCI IDS

 $Me^{-(CH_2)_{19}-Me}$ 

 $H_2N-CH_2-CH_2-NH-CH_2-D1$ 

D1-OH

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 36 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:453155 HCAPLUS

DOCUMENT NUMBER: 79:53155

TITLE: Cyclic amidines. XXV. Derivatives of 1-alkyl-2-amino-4(1H)-quinolinones and

2,3-dihydroimidazo[1,2-a]quinolin-5(1H)-one

AUTHOR(S): Grout, Raymond J.; Hynam, Brian M.; Partridge, Maurice

W.

CORPORATE SOURCE: Dep. Pharm., Univ. Nottingham, Nottingham, UK

SOURCE: Journal of the Chemical Society, Perkin Transactions
1: Organic and Bio-Organic Chemistry (1972-1999) (

**1973**), (12), 1314-20

CODEN: JCPRB4; ISSN: 0300-922X

DOCUMENT TYPE: Journal LANGUAGE: English

GI For diagram(s), see printed CA Issue.

AB Addnl. data considered in abstracting and indexing are available from a source cited in the original document. Fusion of NCCH2CO2Et with N-alkyl arylamine salts gave 1-alkyl-2-amino-4(1H)-quinolinones (I, e.g. R = R1 = Me) which could be O-alkylated to give strong bases. Reaction of PhNH(CH2)2NH2 with EtO2CCH:C(OEt)NH2.HCl gave 2-[(ethoxycarbonyl)-methylene]-1-phenylimidazolidine which cyclized with polyphosphoric acid to 2,3-dihydroimidazo[1,2-a]quinolin-5(1H)-one (II).

IT 42712-72-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 42712-72-1 HCAPLUS

CN 1,2-Ethanediamine, N-phenyl-, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 1664-40-0 CMF C8 H12 N2

PhNH-CH2-CH2-NH2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

HO3S Me

L37 ANSWER 37 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1973:124588 HCAPLUS

DOCUMENT NUMBER: 78:124588
TITLE: Tetramisole

INVENTOR(S): McMinim, Michael Edward

PATENT ASSIGNEE(S): Imperial Chemical Industries Ltd.

SOURCE: Ger. Offen., 50 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2236970	A1	19730208	DE 1972-2236970	19720727 <
GB 1351031	A	19740424	GB 1971-35206	19710727 <
US 3845070	Α	19741029	US 1972-270298	19720710 <
ZA 7204731	Α	19730425	ZA 1972-4731	19720711 <
HU 164067	P	19731228	HU 1972-IE523	19720717 <
AU 7244622	A1	19740124	AU 1972-44622	19720717 <
BE 786416	A1	19730118	BE 1972-119992	19720718 <
DD 103645	C	19740212	DD 1972-164664	19720725 <
FR 2147214	A1	19730309	FR 1972-26901	19720726 <
FR 2147214	B1	19790112		
JP 52029317	B4	19770801	JP 1972-74247	19720726 <
US 3925440	Α	19751209	US 1974-475272	19740531 <
PRIORITY APPLN. INFO.:			GB 1971-35206	A 19710727
			US 1972-270928	A3 19720710

GI For diagram(s), see printed CA Issue.

The title compound (I, R = Ph), useful as an anthelmintic, was prepared by cyclization of II (R1 = e.g. H, Me, Me2CH, Me2CHCH2, Et, CH2:CH:CHCH2, Ph, PhCH2; R2 = H, Ac, Bz, PhCH2CO). II were prepared from HOCHPhCH2NHCH2CH2OH, which was con-verted into R2NHCHPhCH2NHCH2CH2R3 (R2 = SO4H, Cl, Br) (III). III either was treated with R1NCS to give II or it was converted into the corresponding 1-(2-amino-2-phenylethyl)aziridine which on reaction with H2NCSNH2 gave II.

IT 40969-87-7P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 40969-87-7 HCAPLUS

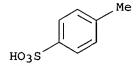
CN 1,2-Ethanediamine, N2-(2-bromoethyl)-1-phenyl-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 48135-01-9 CMF C10 H15 Br N2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S



L37 ANSWER 38 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1970:43001 HCAPLUS

DOCUMENT NUMBER: 72:43001

TITLE: Hydrazine amines with expected antitubercular

activity. V. Synthesis of 2-aminoethylhydrazine and

its derivatives

AUTHOR(S): Grudzinski, Stefan; Kotelko, Antoni; Strumillo, Jozef

CORPORATE SOURCE: Akad. Med., Lodz, Pol.

SOURCE: Acta Poloniae Pharmaceutica (1969), 26(3),

217-22

CODEN: APPHAX; ISSN: 0001-6837

DOCUMENT TYPE: Journal LANGUAGE: Polish

Known synthetic procedures were rechecked; that of Eiter and Truscheit (1961) yielded 42.5% H2NCH2CH2NHNH2 (I) and 17.5% (H2NCH2CH2)2NNH2 (II), whereas that of Kloes and Offe (1960) gave only 23.5% I. The following salts were prepared by routine methods: I.2HCl, m. 169-71°; I dioxalate, m. 196.5-8° (decomposition); I ditartrate, m. 169-71° (70% MeOH); I dipicrate, m. 175-6° (decomposition) (50% MeOH); I bis (benzenesulfonate), decomposition >16°; I bis (p-toluenesulfonate), decomposition >22°; II tripicrate, m. 168-71° (decomposition) (60% MeOH). I and 2.25 moles BzH refluxed a few min in MeOH yielded 67.5% p-RC6H4CH:-NNHCH2CH2N:CHC6H4R-p (III, R = H), b2 204-6°. Analogously was prepared (99.5%) the III (R = NO2), m. 169-70° (Ph nO2). p - O2NC6H4CH:NN(CH2CH2N:CHC6H4NO2 - p)2 (69.5%, m. 176-8° from MeOCH2CH2OH) was prepared similarly from II.

IT 24932-68-1P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 24932-68-1 HCAPLUS

CN Ethanamine, 2-hydrazino-, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 14478-61-6 CMF C2 H9 N3

H2N-CH2-CH2-NH-NH2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L37 ANSWER 39 OF 39 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1969:480815 HCAPLUS

DOCUMENT NUMBER:

71:80815

TITLE:

Therapeutic primary aliphatic diamine salts of

2-oxo-10-bornanesulfonic, 2-oxo-3-bornanecarboxylic,

citric, guaiacylacetic, p-toluenesulfonic, and

benzenesulfonic acids

INVENTOR (S):

Leroi, Eugene L.; Renault, Jean A. Societe d'Etudes de Produits Chimiques

PATENT ASSIGNEE(S): SOURCE:

Belg., 17 pp. CODEN: BEXXAL

DOCUMENT TYPE:

Patent

LANGUAGE:

French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE									
	BE 715739		19681016		<									
	DE 1768656			DE										
	FR 1587351			FR .										
	FR 7959			FR										
	GB 1176077			GB										
PRIC	RITY APPLN. INFO.:			GB	19670612									
AB				cting the acid with										
	temperature in MeOH or H2O. Thus, 225 g. ethylenediamine in 0.5 l. MeOH was													
	slowly added to 1370 g. guaiacylacetic acid in 5 l. MeOH at 25°.													
				oled to precipitate										
				pared were (m.p. giv	ren):									
	ethylenediamine (±)													
	(decomposition); et	hylened	diamine (+)-2	e-oxo-10-bornanesulf	conate, 284°									
	(decomposition); et	nylened	liamine p-to	uenesulionate, 295-	6° (decomposition);									
	215-16° (decomposit			ethylenediamine o	illate,									
				00°); 1,3-diaminopro	nane									
	bornanecarboxyrace,	eculfor	abililled at 20	ecomposition); $1,4-6$	liaminobutane									
	$(\pm)$ -2-0x0-10-bornar $(\pm)$ -2-0x0-10-bornar	esulfor	nate 200 (ue	5-diaminopentane	Taminobutane									
	$(\pm)$ -2-0x0-10-bornar $(\pm)$ -2-0x0-10-bornar	resulto:	nate, 250°, 1	decomposition):										
	1,6-diaminohexane													
				)-2-oxo-10-bornanes	sulfonate.									
	165-7°; 1,8-diamino				,									
	165-7°; 1,9-diamino													
	185-7°; 1,9-diamino													
	157-9°; 1,4-diamino	butane	(+) -2 - 0x0 - 3 - 0	bornanecarboxylate,	(sublimed									
	at 280°); 1,6-diami	inohexaı	ne p-toluenes	sulfonate, 185-7°;										
	1,8-diaminooctane	guaiacy:	lacetate, 136	5°; N,N'-dimethyleth	nylene-									
	diamine $(\pm)$ -2-oxo-1													
				o-10-bornanesulfonat	e									
	170-1°; N,N,N,N-tet													
				; N,N,N,N-tetraethy										
	amine $(\pm)$ -2-oxo-10-	-bornane	esulfonate, 2	233° (decomposition)	<i>;</i>									

N, N-dimethyl-1, 3-propanediamine (±)-2-oxo-10-bornanesulfonate, 193-5°; N,N,N,N-tetramethyl-1,3-propanediamine  $(\pm)$ -2-oxo-10bornanesulfonate, 216°; N,N-dimethyl-1,6-hexanediamine (±)-2-oxo-10-bornanesulfonate, 168°; N,N,N,N-tetramethyl-1,6hexanediamine  $(\pm)$ -2-oxo-10-bornanesulfonate, 108° (decomposition). IT23571-07-5P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) RN23571-07-5 HCAPLUS 1,2-Ethanediamine, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME) CNCM 1 CRN 107-15-3 CMF C2 H8 N2

H2N-CH2-CH2-NH2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

=> 🛚

=> d stat que L9 STR

 $N \sim CH2 - CH \sim NH2$ 1 2 3 4

NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RING(S) ARE ISOLATED OR EMBEDDED NUMBER OF NODES IS 4

STEREO ATTRIBUTES: NONE L10 STR

5 0 ||| N~~ CH2- C~~ NH2 1 2 3 4 NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

**GRAPH ATTRIBUTES:** 

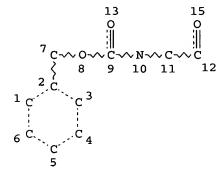
RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 5

STEREO ATTRIBUTES: NONE

L11 7270 SEA FILE=REGISTRY FAM FUL L9
L12 73 SEA FILE=REGISTRY FAM FUL L10

L38 STR



NODE ATTRIBUTES:

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

**GRAPH ATTRIBUTES:** 

RSPEC 2

NUMBER OF NODES IS 14

STEREO ATTRIBUTES: NONE

L40	94241	SEA	FILE=REGISTRY	SSS FUL	L38	
L41	25543	SEA	FILE=REGISTRY	ABB=ON	PLU=ON	TOLUENESULFON?
L42	27708	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L40
L43	82176	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L41
L47	35	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L42 AND TOLUENESULFONIC(L)SALT
L49	17976	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L42(L)REACT?/RL
L53	37642	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L11
L54	1370	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L12
L55	45	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L42 AND L43 AND (L53 OR L54)
L56	20	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L42 AND L43 AND L47
L57	64	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L55 OR L56
L58	41	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L57 AND L49
L59	37	SEA	FILE=HCAPLUS A	BB=ON	PLU=ON	L58 AND PD= <november 2003<="" 5,="" td=""></november>

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=>

=> d ibib abs hitstr 159 1-37

L59 ANSWER 1 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

2004:240415 HCAPLUS

DOCUMENT NUMBER:

140:287714

```
Peptide nucleic acids with N\alpha-(2-aminoethyl)-
TITLE:
                        histidine backbones having enhanced binding affinity
                        and sequence specificity
INVENTOR(S):
                        Nielsen, Peter E.; Egholm, Michael; Berg, Rolf H.;
                        Buchardt, Ole
PATENT ASSIGNEE(S):
                        Den.
                        U.S., 70 pp., Cont.-in-part of U.S. 5,719,262.
SOURCE:
                        CODEN: USXXAM
DOCUMENT TYPE:
                        Patent
                        English
LANGUAGE:
FAMILY ACC. NUM. COUNT:
                        19
PATENT INFORMATION:
    PATENT NO.
                        KIND
                               DATE
                                          APPLICATION NO.
                                                                 DATE
    _____
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                               -----
                                           -----
                                                                  -----
    US 6710164
                         В1
                               20040323
                                        US 1999-230088
                                                                 19990310
    US 6395474
                        B1
                               20020528
                                        US 1993-108591
                                                                 19931122 <--
    US 5773571
                        Α
                               19980630 US 1996-595387
                                                                 19960201 <--
    US 5714331
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                               19980203
                                        US 1996-686116
                                                                 19960724 <--
    US 5719262
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                               19980217
                                          US 1996-685484
                                                                 19960724 <--
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                        Α
                               19980616
                                           US 1996-686113
                                                                 19960724 <--
    US 6414112
                         B1
                               20020702
                                           US 1996-686114
                                                                 19960724 <--
    WO 9803542
                         A1
                               19980129
                                           WO 1997-US12811
                                                                 19970724 <--
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            EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC,
            LK, LR, LS, LT, LU, LV, MD, MG, MN, MW, MX, NO, NZ, PL, PT, RO,
            RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN,
            YU, ZW, AM, AN, BY, KG, KZ, MD, RU, TJ, TM
        RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
            GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
            GN, ML, MR, NE, SN, TD, TG
    US 6107470
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                               20000822
                                           US 1999-225146
                                                                  19990104 <--
PRIORITY APPLN. INFO.:
                                           US 1993-108591
                                                              A2 19931122
                                           US 1996-685484
                                                              A2 19960724
                                           US 1996-686113
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                                                              P 19970529
                                           WO 1997-US12811
                                                              W 19970724
                                           DK 1991-986
                                                              A 19910524
                                           DK 1991-987
                                                              A 19910524
                                           DK 1992-510
                                                              A 19920415
                                           WO 1992-EP1219
                                                              W 19920522
                                           US 1993-54363
                                                              A3 19930426
                                           US 1998-69705
                                                              Al 19980429
                        MARPAT 140:287714
OTHER SOURCE(S):
    Peptide nucleic acid (PNA) monomers comprising N\alpha-(2-aminoethyl)-(D
    or L)-His-OH backbones as well as various derivs. of these monomers are
    disclosed. Replacement of Gly in the classical PNA backbone with His may
    enhance sequence specificity, binding affinity, and/or solubility of the PNA.
    107-15-3, 1,2-Ethanediamine, reactions 2130-76-9
IT
    RL: RCT (Reactant); RACT (Reactant or reagent)
        (peptide nucleic acids with Nα-(2-aminoethyl)-histidine backbones
       having enhanced binding affinity and sequence specificity)
RN
    107-15-3 HCAPLUS
    1,2-Ethanediamine (9CI) (CA INDEX NAME)
CN
```

H2N-CH2-CH2-NH2

RN 2130-76-9 HCAPLUS

CN L-Lysine, N6-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ \text{HO}_2\text{C} & & \\ & &$$

IT 34046-07-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(peptide nucleic acids with N $\alpha$ -(2-aminoethyl)-histidine backbones

having enhanced binding affinity and sequence specificity)

RN 34046-07-6 HCAPLUS

CN Glycine, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-N-

[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} O & \\ | \\ C-O-CH_2-Ph & O \\ | & | \\ | \\ HO_2C-CH_2-N-CH_2-CH_2-NH-C-OBu-t \\ \end{array}$$

REFERENCE COUNT: 167 THERE ARE 167 CITED REFERENCES AVAILABLE FOR

THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE

FORMAT

L59 ANSWER 2 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:583966 HCAPLUS

DOCUMENT NUMBER: 139:277132

TITLE: Synthesis of non-natural amino acids from

N-(p-tolylsulfonyl)-α,β-didehydroamino acid

derivatives

AUTHOR(S): Ferreira, Paula M. T.; Maia, Hernani L. S.; Monteiro,

Luis S.

CORPORATE SOURCE: Departamento de Quimica-Universidade do Minho, Braga,

4710-057, Port.

SOURCE: European Journal of Organic Chemistry (2003

), (14), 2635-2644

CODEN: EJOCFK; ISSN: 1434-193X

PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 139:277132

AB Carbon nucleophiles, amines, and oxygen nucleophiles were treated with the

Me ester of N-(tert-butoxycarbonyl)-N-(p-tolylsulfonyl)- $\alpha$ ,  $\beta$ -

didehydroalanine and also with the Me esters of N-(tert-butoxycarbonyl)-O-(p-tolylsulfinyl)- $\alpha$ ,  $\beta$ -didehydroserine and N-(tert-

butoxycarbonyl)- $\beta$ -(1,2,4-triazol-1-yl)- $\alpha$ , $\beta$ -

didehydroalanine, both of which were obtained from the former substrate.

Carbon nucleophiles of the  $\beta$ -dicarbonyl type gave furanic amino acids, which were converted into the corresponding pyrrole derivs.

(dehydroprolines) in high yields, while use of amines allowed the synthesis of  $\alpha, \alpha$ -diamino acids and  $\beta$ -amino- $\alpha, \beta$ didehydroamino acids. Different types of alkoxyamino acids were obtained by treatment of the above substrates with oxygen nucleophiles. The reactivities of the  $\alpha,\beta$ -didehydroaminobutyric and  $\alpha, \beta$ -didehydrophenylalanine analogs were also tested. Some of the methods developed were applied to the synthesis of cross-linked amino acids, namely didehydrolanthionine and histidino- $\alpha$ ,  $\beta$ didehydroalanine derivs.

107-15-3, Ethylenediamine, reactions 5591-93-5 IT 17136-46-8

> RL: RCT (Reactant); RACT (Reactant or reagent) (synthesis of non-natural amino acids from N-tosyl- $\alpha$ ,  $\beta$ didehydroamino acid derivs.)

107-15-3 HCAPLUS RN

1,2-Ethanediamine (9CI) (CA INDEX NAME) CN

 $H_2N-CH_2-CH_2-NH_2$ 

5591-93-5 HCAPLUS RN

L-Lysine, N2-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX CN NAME)

Absolute stereochemistry.

17136-46-8 HCAPLUS RN

L-Serine, N-[(4-methylphenyl)sulfonyl]-, methyl ester (9CI) (CA INDEX CN NAME)

Absolute stereochemistry.

ΙT 606148-44-1P

> RL: SPN (Synthetic preparation); PREP (Preparation) (synthesis of non-natural amino acids from N-tosyl- $\alpha$ ,  $\beta$ didehydroamino acid derivs.)

RN 606148-44-1 HCAPLUS

CN 13-Oxa-2,8,11-triazapentadecanoic acid, 3,10-bis(methoxycarbonyl)-14,14dimethyl-11-[(4-methylphenyl)sulfonyl]-12-oxo-, phenylmethyl ester, (10S)(9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L59 ANSWER 3 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:485719 HCAPLUS

DOCUMENT NUMBER: 139:53315

TITLE: Preparation of N-sulfonylated dipeptide derivatives as

inhibitors of leukocyte adhesion mediated by VLA-4
Thorsett, Eugene D.; Semko, Christopher M.; Pleiss,
Michael A.; Kreft, Anthony; Konradi, Andrei W.; Grant,

Francine S.; Baudy, Reinhardt Bernhard; Sarantakis,

Dimitrios

PATENT ASSIGNEE(S): USA

SOURCE: U.S., 81 pp., Cont.-in-part of U.S. Ser. No. 127,346,

abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

INVENTOR (S):

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6583139	B1	20030624	US 2000-688820	20001017 <
US 2004006093	A1	20040108	US 2003-382988	20030307
PRIORITY APPLN. INFO.:			US 1997-104592P	P 19970731
			US 1998-127346	B1 19980731
			US 2000-688820	A1 20001017

OTHER SOURCE(S): MARPAT 139:53315

Disclosed are N-sulfonylated dipeptides R1SO2NR2CHR3-Q-CHR5CO2H [R1, R3 = (un)substituted alkyl, aryl, cycloalkyl, heterocyclyl or heteroaryl; R2 = H, (un)substituted cycloalkenyl, or any group given for R1; or R2 may form an (un)substituted heterocyclic ring with R1 or R3; R5 = CH2-X', where X' = H, OH, acylamino, (cyclo)alkyl, alkoxy, aryloxy, (hetero)aryl, aryloxyalkyl, carboxy, carboxyalkyl, etc.; Q = C(X)NR7; R7 = H, alkyl; X = O, S (with provisos)] which bind VLA-4. Certain of these compds. also inhibit leukocyte adhesion and, in particular, leukocyte adhesion mediated by VLA-4. Such compds. are useful in the treatment of inflammatory diseases in a mammalian patient, e.g., human, such as asthma, Alzheimer's disease, atherosclerosis, AIDS dementia, diabetes, inflammatory bowel disease, rheumatoid arthritis, tissue transplantation, tumor metastasis and myocardial ischemia. The compds. can also be administered for the treatment of inflammatory brain diseases such as multiple sclerosis.

Thus, coupling of N-tosyl-L-proline with L-tyrosine Me ester, followed by reaction with (1-bromoethyl)benzene and saponification, afforded N-tosyl-L-prolyl-4-( $\alpha$ -methylbenzyloxy)-L-phenylalanine.

107-15-3, Ethylenediamine, reactions 3886-08-6

51077-01-1 51644-83-8 71449-08-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of N-sulfonylated dipeptide derivs. as inhibitors of leukocyte adhesion mediated by VLA-4)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

 $H_2N - CH_2 - CH_2 - NH_2$ 

IT

RN 3886-08-6 HCAPLUS

Absolute stereochemistry. Rotation (-).

RN 51077-01-1 HCAPLUS

CN L-Proline, 1-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 51644-83-8 HCAPLUS

CN D-Glutamic acid, N-[(phenylmethoxy)carbonyl]-, 5-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 71449-08-6 HCAPLUS

D-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, 4-(1,1-dimethylethyl) ester CN (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

THERE ARE 87 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L59 ANSWER 4 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

87

ACCESSION NUMBER:

2002:107305 HCAPLUS

DOCUMENT NUMBER:

136:172757

TITLE:

Salt forms of an HIV protease inhibitor

INVENTOR(S):

Harris, Gregory D.; Anderson, Stephen R.; Desikan, Sridhar; Meenan, Paul A.; Stone, Benjamin R.; Toma,

Pascal H.

PATENT ASSIGNEE(S):

Dupont Pharmaceuticals Company, USA

SOURCE:

PCT Int. Appl., 56 pp.

CODEN: PIXXD2

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT 1	NO.	KIND		DATE			APPLICATION NO.						DATE				
	<b></b>	_		-	<b>-</b> -												
WO 2002	A2		2002	0207	•	WO 2	001-	US22		20010719 <							
WO 20020		A3		2003	0501												
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	CO, CR	, CU,	CZ,	DE,	DK,	DM,	DZ,	EC,	EE,	ES,	FI,	GB,	GD,	GE,	GH,		
	GM, HR	, HU,	ID,	IL,	IN,	IS,	JP,	KE,	KG,	KP,	KR,	ΚZ,	LC,	LK,	LR,		
	LS, LT	, LU,	LV,	MA,	MD,	MG,	MK,	MN,	MW,	MX,	MZ,	NO,	NZ,	PL,	PT,		
	RO, RU	, SD,	SE,	SG,	SI,	SK,	SL,	ТJ,	TM,	TR,	TT,	TZ,	UA,	UG,	UZ,		
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RW:	GH, GM	, KE,	LS,	MW,	MZ,	SD,	SL,	SZ,	TZ,	UG,	ZW,	AM,	ΑZ,	BY,	KG,		
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	GQ, GW	, ML,	MR,	ΝE,	SN,	TD,	TG										
US 2002	022742		A1		2002	0221		US 2001-908126					20010718 <				

PRIORITY APPLN. INFO.:

US 2000-219794P

Ι

P 20000729

GΙ

AB An HIV protease inhibitor (I) and its salt forms, i.e., mono-fumarate, mono-camphor sulfonate, mono-methane sulfonate, mono-phosphate, and bis-toluene sulfonate, are prepared for pharmaceutical kits useful for treating HIV viral infections. Pharmaceutical kits comprise (a) a salt of I and (b) at least one compound selected from HIV reverse transcriptase inhibitors, such as AZT, efavirenz, and 3TC, and other HIV protease inhibitors, such as saquinavir, ritonavir, nelfinavir and indinavir. Component (a) and component (b) may be sep. or phys. combined into a single dosage form, e.g., a capsule, a suspension, or a parenteral compn.

IT 104-15-4, p-Toluenesulfonic acid, reactions
62965-10-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation and formulation of **salt** forms of HIV protease inhibitor for treatment of HIV viral infections)

RN 104-15-4 HCAPLUS

CN Benzenesulfonic acid, 4-methyl- (9CI) (CA INDEX NAME)

RN 62965-10-0 HCAPLUS

CN L-Valine, 3-methyl-N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 183553-99-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and formulation of salt forms of HIV protease inhibitor for treatment of HIV viral infections)

RN 183553-99-3 HCAPLUS

CN 11-Oxa-2,5,9-triazatridecanoic acid, 3-(1,1-dimethylethyl)-7-hydroxy-12,12-dimethyl-9-(2-methylpropyl)-4,10-dioxo-6-(phenylmethyl)-, phenylmethyl ester, (3S,6S,7R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L59 ANSWER 5 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2000:117072 HCAPLUS

DOCUMENT NUMBER: 132:166522

TITLE: Preparation of depsipeptide derivatives bearing

piperazinone rings as enhancers of apolipoprotein E

production

INVENTOR(S): Yanai, Makoto; Suzuki, Masashi; Oshida, Norio;

Kawamura, Koji; Hiramoto, Shigeru; Yasuda, Orie; Kinoshita, Nobuhiro; Shingai, Akiko; Takasu, Masako

PATENT ASSIGNEE(S): Nisshin Flour Milling Co., Ltd., Japan

SOURCE: PCT Int. Appl., 47 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2000008047 W: JP, US	A1	20000217	WO 1999-JP4205	19990804 <
RW: DE, FR, GB,	IT			
EP 1028126	A1	20000816	EP 1999-935054	19990804 <
R: DE, FR, GB,	IT			
US 6288038	B1	20010911	US 2000-509132	20000403 <
PRIORITY APPLN. INFO.:			JP 1998-220398 A	19980804
			WO 1999-JP4205 W	19990804

OTHER SOURCE(S): MARPAT 132:166522

GΙ

$$\begin{array}{c|c} O & Pr-i \\ \hline \\ NHA^1 \\ \hline \\ Me & 10 \\ \hline \end{array}$$

$$Q = \bigvee_{\substack{N \\ R6}}^{O} \bigvee_{R7}^{N} \bigvee_{O}^{R8}$$

$$Q^{1} = \bigvee_{N}^{N} \bigvee_{R9}^{N} \bigvee_{O}^{R10}$$

AB Novel depsipeptide derivs. bearing piperazinone rings in the mol., represented by general formula R1CH(CH2B)O2CCH(R2)-X1-CH(R3)-A [wherein X1 is N(R4)CO, N(R5)CH2, CH2CO, CH2CH2, CH:CH, CH2CH(OH) or CH(OH)CH(OH); R1 is C5-20 alkyl or C5-15 alkoxy-C1-4 alkyl; R2 to R5 are each hydrogen or C1-6 alkyl; and A is Q, Q1, or -X2-CH(R11)-X3-CH(R12)-NH-R13; wherein X2, X3 = NR14CO, NR15CH2, CH2CO, CH2CH2, CH:CH, CH2 CH(OH), CH(OH)CH(OH); R6, R12, R14, R15 = H, C1-6 alkyl; R7, R9, R11 = (CH2)m1CO2H (wherein m1 = 1-3); R8, R13 = H, amine-protecting group commonly used in peptide chemical; R10 = H, C1-6 alkyl, CO2H, or C1-6 alkoxycarbonyl; B = CO2H, C1-6 alkoxycarbonyl, or Q2; R16 = (CH2)m2CO2H (wherein m2 = 1-3), (CH2)n2CONH2 (wherein n2 = 2,3); R17 = H, C1-6 alkyl, CO2H, C1-6 alkoxycarbonyl] or pharmacol. acceptable salts are prepared as well as pharmaceutical formulations containing them. These derivs. exhibit apolipoprotein E

accelerating activities, thus being useful as remedies for nerve injury, dementia, and hyperlipidemia. Thus, an intermediate (HO-Q3) was condensed with an intermediate (I; R = tert-Bu, A1 = H) using 1-ethyl-3-(3-dimethylaminopropyl)carbodiimide hydrochloride and HOBt in CH2Cl2 under ice-cooling for 2 h and at room temperature overnight to give II (A1 = Q3, R = tert-butyl), which was treated with CF3CO2H to give II (A1 = Q3, R = H). In an enzyme immunoassay using Hep G2 cells, the latter depsipeptide in vitro increased the production of apolipoprotein E by 228 and 458% at 1 and 5  $\mu M$ , resp.

IT 16652-75-8, D-Isoleucine benzyl ester p-toluenesulfonic acid salt 28862-79-5

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of depsipeptide derivs. bearing piperazinone rings as enhancers of apolipoprotein E production for remedies for nerve injury, dementia, and hyperlipidemia)

RN 16652-75-8 HCAPLUS

CN L-Isoleucine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

RN 259087-04-2 HCAPLUS

CN 3,11-Dioxa-5,8-diazatetradecan-14-oic acid, 2,2-dimethyl-9-[(1R)-1-methylpropyl]-6-(2-methylpropyl)-4,10-dioxo-8-[(phenylmethoxy)carbonyl]-12-undecyl-, phenylmethyl ester, (6R,9R,12R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 259087-05-3 HCAPLUS

CN D-Isoleucine, N-[(2R)-2-amino-4-methylpentyl]-N-[(phenylmethoxy)carbonyl]-, (1R)-1-[2-oxo-2-(phenylmethoxy)ethyl]dodecyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

CM 1

CRN 42406-72-4 CMF C13 H19 N O2

Absolute stereochemistry.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 28862-79-5 HCAPLUS

CN D-Leucine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 259087-03-1P 259087-04-2P 259087-05-3P

259087-06-4P 259087-18-8P 259087-19-9P

259087-20-2P 259087-21-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of depsipeptide derivs. bearing piperazinone rings as enhancers of apolipoprotein E production for remedies for nerve injury, dementia, and hyperlipidemia)

RN 259087-03-1 HCAPLUS

CN D-Isoleucine, N-[(2R)-2-[[(1,1-dimethylethoxy)carbonyl]amino]-4methylpentyl]-N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 259087-06-4 HCAPLUS

CN 1-Piperazinepropanoic acid, 4-[(9H-fluoren-9-ylmethoxy)carbonyl]-β[(3R,6R,9R)-6-[(1R)-1-methylpropyl]-3-(2-methylpropyl)-1,7,11-trioxo-13phenyl-5-[(phenylmethoxy)carbonyl]-9-undecyl-8,12-dioxa-2,5-diazatridec-1yl]-2-oxo-, 1,1-dimethylethyl ester, (βS)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 2-A

RN 259087-18-8 HCAPLUS

CN Heptanoic acid, 6-methyl-3-oxo-4-[[(phenylmethoxy)carbonyl]amino]-, 1,1-dimethylethyl ester, (4R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 259087-19-9 HCAPLUS

CN Octanoic acid, 7-methyl-4-oxo-5-[[(phenylmethoxy)carbonyl]amino]-, methyl ester, (5R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 259087-20-2 HCAPLUS

CN Octanoic acid, 7-methyl-4-oxo-5-[[(phenylmethoxy)carbonyl]amino]-, (5R)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 259087-21-3 HCAPLUS

CN Tetradecanoic acid, 3-[[(5R)-7-methyl-1,4-dioxo-5-[[(phenylmethoxy)carbonyl]amino]octyl]oxy]-, 1,1-dimethylethyl ester, (3R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L59 ANSWER 6 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

2000:68440 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 132:122633

TITLE: Substituted piperazinones and their therapeutic uses

as antithrombotics

INVENTOR(S): Yue, Christophe; Henry, Marguerite; Giboulot, Thierry;

Lesur, Brigitte

PATENT ASSIGNEE(S): Laboratoire L. Lafon, Fr. SOURCE: PCT Int. Appl., 52 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PA										APPLICATION NO.									
WO	2000	0040	01		A1		2000	0127	WO 1999-FR1751						19990716 <				
											BR,								
							-	-		-	GM,	-		•					
											LS,								
							-	-		-	SD,		-	•		•			
											ZA,								
		•	RU,	•		,	,	02,	,	10,	2,	,	,	112,	21,	1.0,	,		
	RW:	•	•	•		MW.	SD.	SL.	SZ.	UG.	ZW,	AT.	BE.	CH.	CY.	DE.	DK.		
•											NL,								
			-	-		-	-	-			TD,			22,	20,	01,	00,		
FR	2781										998-				1	9980	717	<	
	2781														_			•	
								CA 1999-2337880						1	9990	716	< <b>-</b> -		
	9946							AU 1999-46293											
AU	7519	81			B2 20020905														
									BR 1999-12153						19990716 <				
	1098																		
											IT,								
							RO		,	0,	,	,	20,	112,	02,	,	,		
ďΡ	2002									TP 2	000-	5601	n a		1	9990	716	<	
	5091																		
	6335															0010			
PRIORITY					<i></i> 1		2002	0101			998-								
INIONII	. AFF.	HI	1141.0	• •							999-					9990			
OTHER SO	OURCE	(s):			MARI	PAT	132:	1226			. , , , ,	PKI/	<i>.</i> , T	1	м т	J J J U	, 10		

OTHER SOURCE(S): MARPAT 132:122633 GΙ

$$\begin{array}{c|c}
R^2 - N \\
R^4 - N \\
R^5
\end{array}$$

$$\begin{array}{c|c}
N \\
N \\
\end{array}$$

$$\begin{array}{c}
N \\
\end{array}$$

$$\begin{array}{c}
N \\
\end{array}$$

$$\begin{array}{c}
N \\
\end{array}$$

$$\begin{array}{c}
N \\
\end{array}$$

The invention concerns compds. I [R1 = H, alkyl, phenylalkyl; R2 = H, OH, or protecting group for amidino; R3 = NHCOR6, NHSO2R7; R4, R5 = H, alkyl; or NR4R5 = piperidino or morpholino; R6 = alkoxy, cycloalkoxy, benzyloxy, (di)methoxyphenyl, benzodioxolyl, benzodioxanyl; R7 = (un)substituted alkyl, cycloalkyl, (un)substituted (hetero)aryl, phenylalkyl, naphthylalkyl, indanyl or analogs] and their pharmaceutically acceptable salts. The compds. are useful in therapy as antithrombotic agents. Prepns. of approx. 40 invention compds. and approx. 40 intermediates are described. For example, 2-[4-(4-cyanophenyl)-2-oxopiperazino]acetic acid underwent amidation with (2S)-Et 3-amino-2-[(phenylsulfonyl)amino]propanoa te-HCl (70%), followed by conversion of the nitrile to an amidoxime (78%), and hydrogenolysis of this to an amidine (80%), to give title compound II as the acetate salt. At 10 mg/kg i.g. in guinea pigs, II.HOAc gave 37% inhibition of platelet aggregation after 1 h.

IT 256344-36-2P

RN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(intermediate; preparation of substituted piperazinones as antithrombotics) 256344-36-2 HCAPLUS

CN L-Alanine, 3-[[[4-(4-cyanophenyl)-2-oxo-1-piperazinyl]acetyl]amino]-N[(phenylmethoxy)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 107-15-3, Ethylenediamine, reactions 21753-19-5
167937-59-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(starting material; preparation of substituted piperazinones as antithrombotics)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

H2N-CH2-CH2-NH2

RN 21753-19-5 HCAPLUS

CN L-Alanine, 3-amino-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

$$\begin{array}{c|c} H & & Me \\ H_2N & & S & N \\ HO_2C & O & O \end{array}$$

RN 167937-59-9 HCAPLUS

CN L-Alanine, 3-amino-N-[(phenylmethoxy)carbonyl]-, ethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

HCl

IT 256384-94-8P, CRL 42771

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(target compound; preparation of substituted piperazinones as

antithrombotics)

RN 256384-94-8 HCAPLUS

CN L-Alanine, 3-[[[4-[4-[(hydroxyamino)iminomethyl]phenyl]-2-oxo-1piperazinyl]acetyl]amino]-N-[(phenylmethoxy)carbonyl]-, ethyl ester (9CI)
(CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L59 ANSWER 7 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:509180 HCAPLUS

DOCUMENT NUMBER: 129:161414

TITLE: Preparation of benzamidine derivatives as

anticoagulants

INVENTOR(S): Takayanagi, Masaru; Sagi, Kazuyuki; Nakagawa,

Tadakiyo; Yamanashi, Masahiro; Kayahara, Takashi;

Takehana, Shunji; et al.

PATENT ASSIGNEE(S): Ajinomoto Co., Inc., Japan

SOURCE: PCT Int. Appl., 453 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.						KIND DATE				APPLICATION NO.						DATE			
	WO	9831661			A1	A1 19980723			7	<b>VO</b> 19	998-	JP17		19980119 <						
		W:	AL,	AM,	AT,	AU,	ΑZ,	BA,	BB,	BG,	BR,	BY,	CA,	CH,	CN,	CU,	CZ,	DE,		
			DK,	EE,	ES,	FI,	GB,	GE,	GH,	GM,	GW,	HU,	ID,	IL,	IS,	JP,	KE,	KG,		
			KR,	KZ,	LC,	LK,	LR,	LS,	LT,	LU,	LV,	MD,	MG,	MK,	MN,	MW,	MX,	NO,		
			ΝZ,	PL,	PT,	RO,	RU,	SD,	SE,	SG,	SI,	SK,	SL,	TJ,	TM,	TR,	TT,	UA,		
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	ΑU	9854	975			A1	1 19980807			AU 1998-54975					19980119 <					
	ΑU	7318	19			B2		2001	0405											
	ΕP	9767	22			A1		2000	0202	]	EP 1	998-	9004	22		13	9980	119 <	:	
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PRIOF	(TIS	APP	LN.	INFO	.:						JP 1:	997-	6783		i	A 1:	9970	117		
											JP 1:	997-	1946	02	1	A 1:	9970	718		
											JP 1:	997-	3318	87	1	A 1:	99712	202		
										1	WO 1	998-	JP17	6	1	W 1:	9980	119		

OTHER SOURCE(S): MARPAT 129:161414

GI

The title compds. I [L = CH2CH2, NWCOCH2, etc.; W = H, alkyl, etc.; Y = CH:CH, CONH, etc.; Z = H, alkyl, halo, etc.; when L is CH2CH2, V is benzoyl, cinnamoyl, etc., having substituents; further details on V are given] are prepared These compds. show anticoagulant effects based on their excellent effects of inhibiting activated blood coagulation factor X, which makes them useful as anticoagulants. In in vitro tests for the inhibition of activated blood coagulation factor X, compds. of this invention showed pIC50 values of 5.5 to 8.1.

IT 210959-63-0P 210959-65-2P 210959-67-4P 210959-71-0P 210959-73-2P 210959-75-4P 210959-77-6P 210959-79-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of benzamidine derivs. as anticoagulants)

RN 210959-63-0 HCAPLUS

CN Carbamic acid, [(1R)-2-[[3-[3-(aminoiminomethyl)phenoxy]propyl]amino]-1-methyl-2-oxoethyl]-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA

INDEX NAME)

CM 1

CRN 210959-62-9 CMF C21 H26 N4 O4

Absolute stereochemistry.

Ph O NH H NH 
$$(CH_2)_3$$
 NH  $NH_2$ 

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 210959-65-2 HCAPLUS

CN Carbamic acid, [(1S)-2-[[3-[3-(aminoiminomethyl)phenoxy]propyl]amino]-1-methyl-2-oxoethyl]-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 210959-64-1 CMF C21 H26 N4 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 210959-67-4 HCAPLUS

CN Pentanoic acid, 5-[[3-[3-(aminoiminomethyl)phenoxy]propyl]amino]-5-oxo-4[[(phenylmethoxy)carbonyl]amino]-, (4S)-, mono(trifluoroacetate) (9CI)
(CA INDEX NAME)

CM 1

CRN 210959-66-3 CMF C23 H28 N4 O6

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 210959-71-0 HCAPLUS

CN Carbamic acid, [(1S)-2-[[3-[3-(aminoiminomethyl)phenoxy]propyl]amino]-1 (1H-imidazol-4-ylmethyl)-2-oxoethyl]-, phenylmethyl ester,
 bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 210959-70-9 CMF C24 H28 N6 O4 Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 210959-73-2 HCAPLUS

CN Carbamic acid, [(1S,2S)-1-[[[3-[3-(aminoiminomethyl)phenoxy]propyl]amino]c arbonyl]-2-methylbutyl]-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 210959-72-1 CMF C24 H32 N4 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 210959-75-4 HCAPLUS

CN Carbamic acid, [(1S)-5-amino-1-[[[3-[3-(aminoiminomethyl)phenoxy]propyl]am ino]carbonyl]pentyl]-, phenylmethyl ester, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 210959-74-3 CMF C24 H33 N5 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 210959-77-6 HCAPLUS

CN Carbamic acid, [(1S)-2-[[3-[3-(aminoiminomethyl)phenoxy]propyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 210959-76-5 CMF C27 H30 N4 O4 Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

RN 210959-79-8 HCAPLUS

CN Carbamic acid, [(1R)-2-[[3-[3-(aminoiminomethyl)phenoxy]propyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, mono(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 210959-78-7 CMF C27 H30 N4 O4

Absolute stereochemistry.

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 107-15-3, 1,2-Ethanediamine, reactions 1161-13-3, N-Benzyloxycarbonyl-L-phenylalanine 1939-99-7, 3886-08-6 26607-51-2, N-Benzyloxycarbonyl-D-alanine 210964-08-2 RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of benzamidine derivs. as anticoagulants) 107-15-3 HCAPLUS

RN

CN1,2-Ethanediamine (9CI) (CA INDEX NAME)

$$H_2N-CH_2-CH_2-NH_2$$

1161-13-3 HCAPLUS CN L-Phenylalanine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

1939-99-7 HCAPLUS RN

Benzenemethanesulfonyl chloride (9CI) (CA INDEX NAME) CN

RN2448-45-5 HCAPLUS

D-Phenylalanine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME) CN

Absolute stereochemistry. Rotation (-).

RN 3160-59-6 HCAPLUS

CN L-Isoleucine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 3886-08-6 HCAPLUS

Absolute stereochemistry. Rotation (-).

RN 26607-51-2 HCAPLUS

CN D-Alanine, N-[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 210964-08-2 HCAPLUS

CN Carbamic acid, [(1R)-2-[[3-[3-(aminoiminomethyl)phenoxy]propyl]amino]-2-oxo-1-(phenylmethyl)ethyl]-, phenylmethyl ester, bis(trifluoroacetate) (9CI) (CA INDEX NAME)

CM 1

CRN 210959-78-7

CMF C27 H30 N4 O4

CM 2

CRN 76-05-1 CMF C2 H F3 O2

IT 41888-70-4P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of benzamidine derivs. as anticoagulants)

RN 41888-70-4 HCAPLUS

CN L-Histidine, 1-[(4-methylphenyl)sulfonyl]-N-[(phenylmethoxy)carbonyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

REFERENCE COUNT:

14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L59 ANSWER 8 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:474388 HCAPLUS

DOCUMENT NUMBER: 129:149243

TITLE: Oxidation-induced acyl group transfer from

hydroquinone esters to nucleophiles

AUTHOR(S): Reischl, Gerald; El-Mobayed, Medhat; Beisswenger,

Rudolf; Regier, Klaus; Maichle-Moessmer, Caecilia;

Rieker, Anton

CORPORATE SOURCE: Institute Organic Chemistry, University Tuebingen,

Tuebingen, D-72076, Germany

SOURCE: Zeitschrift fuer Naturforschung, B: Chemical Sciences

**(1998)**, 53(7), 765-773

CODEN: ZNBSEN; ISSN: 0932-0776

PUBLISHER: Verlag der Zeitschrift fuer Naturforschung

DOCUMENT TYPE: Journal LANGUAGE: English

AB Bivalent oxidation of 3,5-di-tert-butylhydroquinone monoesters leads to phenoxenium ions, which can transfer an acyl group to nucleophiles. Based on this principle, dipeptides, glyco amino acids, and N-sulfonyl amino acids were synthesized from hydroquinone esters of amino acids and 4-toluenesulfonic acid. For this reaction, direct anodic and indirect mediated oxidation, as well as chemical oxidation with NBS or trisarylammonium salts was used. The mechanism of the acyl transfer is discussed in terms of a direct and/or mediated process.

IT 1138-80-3 14694-46-3 15030-72-5, Cbz-Aib-OH

210840-42-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of dipeptides, glyco amino acids, and N-sulfonyl amino acids by oxidation-induced acyl transfer from hydroquinone esters)

RN 1138-80-3 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

RN 14694-46-3 HCAPLUS

CN 1,4-Benzenediol, 2,6-bis(1,1-dimethylethyl)-, 4-(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

RN 15030-72-5 HCAPLUS

CN Alanine, 2-methyl-N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{NH-C-O-CH}_2 - \text{Ph} \\ \parallel \\ \text{Me-C-CO}_2 \text{H} \\ \parallel \\ \text{Me} \end{array}$$

RN 210840-42-9 HCAPLUS

CN L-Alanine, N-[(phenylmethoxy)carbonyl]-, 3,5-bis(1,1-dimethylethyl)-4hydroxyphenyl ester (9CI) (CA INDEX NAME)

IT 210840-41-8P 210840-43-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of dipeptides, glyco amino acids, and N-sulfonyl amino acids by oxidation-induced acyl transfer from hydroquinone esters)

RN 210840-41-8 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]-, 3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl ester (9CI) (CA INDEX NAME)

$$Ph-CH_2-O-C-NH-CH_2-C-O$$
 $t-Bu$ 

RN 210840-43-0 HCAPLUS

CN Alanine, 2-methyl-N-[(phenylmethoxy)carbonyl]-, 3,5-bis(1,1-dimethylethyl)-4-hydroxyphenyl ester (9CI) (CA INDEX NAME)

IT 2483-51-4P 2503-32-4P, Cbz-Ala-Gly-OEt

3350-42-3P 7352-21-8P 41041-70-7P,

Cbz-Ala-Leu-OEt 84758-85-0P 210840-44-1P

210840-46-3P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of dipeptides, glyco amino acids, and N-sulfonyl amino acids by oxidation-induced acyl transfer from hydroquinone esters)

RN 2483-51-4 HCAPLUS

Absolute stereochemistry.

RN 2503-32-4 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]-L-alanyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 3350-42-3 HCAPLUS

CN L-Alanine, 2-methyl-N-[(phenylmethoxy)carbonyl]alanyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 7352-21-8 HCAPLUS

CN L-Leucine, N-[(phenylmethoxy)carbonyl]glycyl-, ethyl ester (9CI) (CA INDEX NAME)

RN 41041-70-7 HCAPLUS

CN L-Leucine, N-[(phenylmethoxy)carbonyl]-L-alanyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 84758-85-0 HCAPLUS

Absolute stereochemistry.

RN 210840-44-1 HCAPLUS

CN L-Alanine, N-[(phenylmethoxy)carbonyl]-, ester with methyl 2,3-0-(1-methylethylidene)-β-D-ribofuranoside (9CI) (CA INDEX NAME)

RN 210840-46-3 HCAPLUS

CN L-Leucine, 2-methyl-N-[(phenylmethoxy)carbonyl]alanyl-, ethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L59 ANSWER 9 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:441926 HCAPLUS

DOCUMENT NUMBER: 129:122864

TITLE: Preparation of peptide nucleic acids having enhanced

binding affinity and sequence specificity

INVENTOR(S): Burchardt, Ole; Egholm, Michael; Nielsen, Peter Eigil;

Berg, Rolf Henrik; Burchardt, Dorte

PATENT ASSIGNEE(S): Isis Pharmaceuticals, Inc., Den.

SOURCE: U.S., 72 pp., Cont.-in-part of U.S. Ser. No. 108,591.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 19

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
US 5766855	A 19980616	US 1996-686113	19960724 <
CA 2109320	AA 19921125	CA 1992-2109320	19920522 <
CA 2109320	C 20030722		
AU 9218806	A1 19921230	AU 1992-18806	19920522 <
AU 666480	B2 19960215		
JP 06509063	T2 19941013	JP 1992-510139	19920522 <
EP 586618	B1 19970716	EP 1992-923579	19920522 <
EP 586618	A1 19940316		
R: AT, BE, CH,	DE, DK, ES, FR,	GB, GR, IT, LI, LU, NL,	SE
EP 1074559	A1 20010207	EP 2000-203148	19920522 <
R: AT, BE, CH,	DE, DK, ES, FR,	GB, GR, IT, LI, LU, NL,	SE, MC
EP 1162206	A2 20011212	EP 2001-203303	19920522 <
EP 1162206	A3 20040414		

AB A novel peptide nucleic acids I [each L = naturally occurring and non-naturally occurring nucleobase, with the proviso that at least one L = 2,6-diaminopurine; each R7 = H, C1-8 alkylamine; R = OH, NH2, NH-Lys-NH2; R1 = H, Ac, Me3CO2C (Boc); n = 1-30] bind complementary DNA and RNA strands more strongly than a corresponding DNA strand, and exhibit increased sequence specificity and binding affinity. Methods of increasing binding affinity and sequence specificity of peptide nucleic acids are provided wherein some peptide nucleic acids comprise ligands selected from a group consisting of naturally-occurring nucleobases and non-naturally-occurring nucleobases attached to a polyamide backbone, while other peptide nucleic acids contain at least one 2,6-diaminopurine nucleobase and at least one C1 -C8 alkylamine side chain. A variety of peptide nucleic acid containing 2,6-diaminopurine and alkylamine side chains were prepared and exhibited enhanced sequence selectivity and binding affinities with complementary DNA and RNA strands.

IT 107-15-3, 1,2-Ethanediamine, reactions 2130-76-9

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of peptide nucleic acids having enhanced binding affinity and sequence specificity)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

H2N-CH2-CH2-NH2

RN 2130-76-9 HCAPLUS

CN L-Lysine, N6-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ \text{HO}_2\text{C} & & \\ & &$$

IT 34046-07-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of peptide nucleic acids having enhanced binding affinity and sequence specificity)

RN 34046-07-6 HCAPLUS

CN Glycine, N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]-N[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC
                                               JP 2003-15384
EP 2003-77836
     JP 2003235590
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WO 1997-US12811
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     WO 9803542
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              GN, ML, MR, NE, SN, TD, TG
     AU 9738081
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                                                AU 1997-38081
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                                               EP 1997-935053 19970724 <--
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                             A1
                                    19991201
          R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
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     US 6710164
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A3 1992055
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PRIORITY APPLN. INFO.:
                                                  DK 1991-987
                                                  DK 1992-510
                                                  US 1993-108591
                                                  EP 1992-911165
                                                  EP 2000-203148
                                                                        A3 19920522
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                                                                         A3 19920522
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                                                                         W 19920522
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                                                                        A 19920522
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OTHER SOURCE(S): MARPAT 129:122864
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Page 113

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$$\begin{array}{c} \text{O} \\ \parallel \\ \text{C-O-CH}_2\text{-Ph} & \text{O} \\ \parallel \\ \text{HO}_2\text{C-CH}_2\text{-N-CH}_2\text{-CH}_2\text{-NH-C-OBu-t} \end{array}$$

REFERENCE COUNT:

157 THERE ARE 157 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L59 ANSWER 10 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:163612 HCAPLUS

DOCUMENT NUMBER: 128:230695

TITLE: Preparation of novel peptide derivatives having

thiazolyl-alanine residue

INVENTOR(S): Sugawara, Tamio; Yoshikawa, Takayoshi; Tada, Yukio

PATENT ASSIGNEE(S): Shionogi & Co., Ltd., Japan

SOURCE: PCT Int. Appl., 139 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

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PRIORITY	Y APP	LN.	INFO	. :					ن	JP 1	996-:	2263	86	i	A 1	9960	828	
									ز	JP 1	997-	9052	9	2	A 1	9970	409	
													17		W 1	9970	822	
OMITTED OF	NTD OD	(0)				~ ~ ~	100					_						

OTHER SOURCE(S): MARPAT 128:230695

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\* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT \*

AB Peptide derivs. represented by general formula [I; A = 4- or 5-thiazolyl; Y = single bond, O, S; m = 0-4; Y = (un)substituted alkyl or CO2H, cyano, CONR1R2; wherein R1, R2 = H or (un) substituted alkyl or NR1R2 = (un) substituted nonarom. heterocyclyl optionally containing O, N, or S; Z = Q, Q1; R3 = H, (un) substituted alkyl, CO2H, or acyl; R4, R5 = H, (un) substituted alkyl; W = (CH2)n, O, S, (un) substituted NH; wherein n =0, 1, 2, or 3] or pharmacol. acceptable salts or hydrates thereof are prepared These peptide compds. have improved central nerve activating effects such as sustained acetylcholine-releasing effect, antireserpine effect and spontaneous motility increasing effect as compared with the publicly known TSH releasing hormone TSH-releasing hormone (TRH) (H-pGlu-His-Pro-NH2) and TRH derivs. Thus, L-pyroglutamic acid was condensed with 3-(4-thiazolyl)-L-alanyl-L-prolinamide hydrochloride using DCC and N-hydroxysuccinimide in DMF to give the title compound (II; R = Q2). II (R = Q3) at 24 µmol/kg p.o. increased ≤260% release of acetylcholine from brain in rat 350 h after administration of the compound TΤ 88035-94-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of novel peptide derivs. having thiazolylalanine residue as central nerve activators)

RN 88035-94-3 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]-, tetradecyl ester (9CI) (CA INDEX NAME)

IT 1138-80-3 204387-55-3, (R)-(+)-2-Methylpyrrolidine ptoluenesulfonic acid salt

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of novel peptide derivs. having thiazolylalanine residue as central nerve activators with sustained acetylcholine-releasing effect, antireserpine effect and spontaneous motility increasing effect)

RN 1138-80-3 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

RN 204387-55-3 HCAPLUS

CN Pyrrolidine, 2-methyl-, (2R)-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 41720-98-3 CMF C5 H11 N

Absolute stereochemistry. Rotation (-).

2 CM

CRN 104-15-4 CMF C7 H8 O3 S

THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 14 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L59 ANSWER 11 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

1997:579696 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 127:228839

Pharmaceutical agents containing perfluoroalkyl-TITLE:

containing metal complexes and the use thereof in

tumor therapy and intervention al radiology

Platzek, Johannes; Niedballa, Ulrich; Raduchel, Bernd; INVENTOR(S):

Schlecker, Wolfgang; Weinmann, Hanns-Joachim; Frenzel,

Thomas

PATENT ASSIGNEE(S): Schering A.-G., Germany

PCT Int. Appl., 144 pp. SOURCE:

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.			KIND	DATE	APPLICATION NO.	DATE
<b>W</b> :	AL, AM JP, KE	, AU, , KG,	AZ, I KP, I	BB, BG, BR, KR, KZ, LK,	WO 1997-EP684 BY, CA, CN, CZ, EE, LR, LS, LT, LV, MD, SG, SI, SK, TJ, TM,	GE, HU, IL, IS, MG, MK, MN, MW,
DE 19608 CA 22472 AU 97176 EP 88203	AT, BE 3278 253 592		A1 AA A1 A1	19970828 19970828 19970910	FR, GB, GR, IE, IT, DE 1996-19608278 CA 1997-2247253 AU 1997-17692 EP 1997-903278	19960223 < 19970214 < 19970214 <
	AT, BE IE, FI	, СН,	DE, 1	DK, ES, FR,	GB, GR, IT, LI, LU,	NL, SE, MC, PT,
JP 20005 AT 20089 ES 21584 PT 88201	504736 94 193		E T3	20000418 20010515 20010901 20011030	JP 1997-529766 AT 1997-903278 ES 1997-903278 PT 1997-903278	19970214 < 19970214 <

20010130 US 6180113 B1 US 1997-801983 19970219 <--ZA 9701537 Α 19971030 ZA 1997-1537 19970221 <--В TW 477699 20020301 TW 1997-86102174 19970222 <--NO 9803875 Α 19981022 NO 1998-3875 19980821 <--Т3 GR 2001-401156 GR 3036306 20011031 20010731 <--PRIORITY APPLN. INFO.: DE 1996-19608278 A 19960223 US 1996-12506P P 19960229 WO 1997-EP684 W 19970214

OTHER SOURCE(S): MARPAT 127:228839

AB The invention relates to pharmaceutical agents containing perfluoro alkylated metal complexes RF-L-A and the use thereof in tumor therapy and interventional radiol., in which formula RF is a perfluorinated, straight-chain or branched C chain with the formula -CnF2nX (X = terminal F, Cl, Br, I or H atom and n = 4-30), L is a binding group, and A is a metal complex or the salts thereof of organic and/or inorg. bases or amino acids or amino acid amides. Thus Gd/Dy/Y/Mn complexes of tetraazacyclododecane having amide pendants with perfluoroalkyl groups or polyaminopolycarboxylic acids with pendants containing perfluoroalkyl groups were prepared

IT 98-59-9, p-Toluenesulfonyl chloride 107-15-3,

1,2-Ethanediamine, reactions 1138-80-3, Benzyloxycarbonylglycine

1738-76-7, Glycine benzyl ester p-toluenesulfonate

2566-20-3, N-Benzyloxycarbonyltriglycine

RL: RCT (Reactant); RACT (Reactant or reagent)

(for preparation of rare earth/manganese fluoroalkyl-containing polyaminopolycarboxylate/tetraazacyclododecane complexes for use as pharmaceutical agents in tumor therapy and interventional radiol.)

RN 98-59-9 HCAPLUS

CN Benzenesulfonyl chloride, 4-methyl- (9CI) (CA INDEX NAME)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

 $H_2N-CH_2-CH_2-NH_2$ 

RN 1138-80-3 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

RN 1738-76-7 HCAPLUS

CN Glycine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 1738-68-7 CMF C9 H11 N O2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 2566-20-3 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]glycylglycyl- (9CI) (CA INDEX NAME)

IT 51740-38-6P 193530-01-7P 193530-05-1P

193530-10-8P 195047-12-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(for preparation of rare earth/manganese fluoroalkyl-containing polyaminopolycarboxylate/tetraazacyclododecane complexes for use as pharmaceutical agents in tumor therapy and interventional radiol.)

RN 51740-38-6 HCAPLUS

CN 1-Octanol, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

RN 193530-01-7 HCAPLUS

CN 11-Oxa-2,5,8-triazaheneicosanoic acid, 14,14,15,15,16,16,17,17,18,18,19,19,20,20,21,21,21-heptadecafluoro-4,9-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-B

- сн $_2$ - Рh

RN 193530-05-1 HCAPLUS

RN 193530-10-8 HCAPLUS

CN Carbamic acid, [2-[4-[(heptadecafluorooctyl)sulfonyl]-1-piperazinyl]-2oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$F_3C-(CF_2)_7-S$$

RN 195047-12-2 HCAPLUS

CN Nonanoic acid, N-[(phenylmethoxy)carbonyl]glycylglycylglycyl-2-amino-4,4,5,5,6,6,7,7,8,8,9,9,9-tridecafluoro-(9CI) (CA INDEX NAME)

L59 ANSWER 12 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:500179 HCAPLUS

DOCUMENT NUMBER: 127:122137

TITLE: Nitrogen-containing cascade polymer transition metal

complexes and their manufacture and use in pharmaceuticals and diagnostic agents

Schmitt-Willich, Heribert; Platzek, Johannes;

Raduechel, Bernd; Weinmann, Hanns joachim; Ebert, Wolfgang; Misselwitz, Bernd; Muehler, Andreas;

Frenzel, Thomas

Schering A.-G., Germany PATENT ASSIGNEE(S): SOURCE:

Ger. Offen., 51 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

INVENTOR(S):

									APPLICATION NO.							DATE			
DE	19549286			A1		19970626			)E 1	995-	19951222 <								
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CZ	294238			В6		2004	1110						19961129						
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PRIORITY	Y APPLN.	INFO	.:							995-									
								W	10 1	996-	EP53	15	1	W 1	9961	129			

Complexes containing (a) A[X[Y[Z(WKw)z]y]x]a ligands (A = N-containing cascade AB polymer core with a branching degree, X, Y = direct bond or repeating unit with branching degree x, y, resp., Z, W = repeating unit with branching degree z, w, resp., K = complex formers, a = 2-12, x, y, z, w = 1-4, ≥2 repeating units being different, 16 ≤ axyzw ≤ 64, and ≥1 of X, Y, Z, W being a 1,4,7,10-tetraazacyclododecane or 1,4,8;11-tetraazacyclotetradecane repeating unit), (b)  $\geq$ 16 ions of metals with atom. nos. 20-29, 39, 42, 44, or 57-83, (c) optionally, an cation of (in)organic base, amino acid, or amino amide, and (d) optionally, acylated terminal amino group are are manufactured for use as pharmaceuticals and contrast agents in NMR tomog. and radiog. A typical complex was manufactured by reaction of HBr with benzyloxycarbonyl-blocked 36mer cascade polyamine prepared from N,N,N',N',N'',N''-hexakis(2-aminoethyl)trimesic acid

core and 6 1-[5-(4-nitrophenoxy)-3-oxaglutaryl]-4,7,10-tris(N,N'dibenzyloxycarbonyllysyl)-1,4,7,10-tetraazacyclododecane, reaction of the resulting 36-mer amine hydrobromide with 1-(3-aza-4-carboxy-2-oxobutyl)-4,7,10-tris(tert-butoxycarbonylmethyl)-1,4,7,10-tetraazacyclododecane, and complexation of the Na salt of the resulting ligand with Gd203. IT 192635-84-0P 192635-85-1P 192635-86-2P 192636-02-5P 192636-03-6P 192636-04-7P 192636-05-8P 192636-26-3P 192636-27-4P 192636-28-5P 192636-29-6P RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (cascade polymer precursor; nitrogen-containing cascade polymer transition metal complexes and their manufacture and use in pharmaceuticals and diagnostic agents) RN192635-84-0 HCAPLUS CN Carbamic acid, [1,4,7,10-tetraazacyclododecane-1,4,7-triyltris[(2S)-1-oxo-1,2,6-hexanetriyl]]hexakis-, hexakis(phenylmethyl) ester (9CI) (CA INDEX

Absolute stereochemistry.

NAME)

PAGE 1-B

RN 192635-85-1 HCAPLUS

CN Acetic acid, [2-oxo-2-[4,7,10-tris[1-oxo-2,6-bis[[(phenylmethoxy)carbonyl] amino]hexyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]-, [2S-[1(R\*),1(R\*),2R\*]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 192635-86-2 HCAPLUS

CN Acetic acid, [2-oxo-2-[4,7,10-tris[1-oxo-2,6-bis[[(phenylmethoxy)carbonyl] amino]hexyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]-, 4-nitrophenyl ester, [2S-[1(R\*),1(R\*),2R\*]]- (9CI) (CA INDEX NAME)

PAGE 1-B

\_\_\_\_ Ph

RN 192636-02-5 HCAPLUS

CN Carbamic acid, [1,4,7,10-tetraazacyclododecane-1,4,7-triyltris(2-oxo-2,1-ethanediyl)]tris-, tris(phenylmethyl) ester (9CI) (CA INDEX NAME)

RN 192636-03-6 HCAPLUS

CN Acetic acid, [2-oxo-2-[4,7,10-tris[[[(phenylmethoxy)carbonyl]amino]acetyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]- (9CI) (CA INDEX NAME)

RN 192636-04-7 HCAPLUS

CN 2,9,12,15,22-Pentaazatricosanedioic acid, 8,16-dioxo-7,17bis[[(phenylmethoxy)carbonyl]amino]-, bis(phenylmethyl) ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

PAGE 1-B

RN 192636-05-8 HCAPLUS
CN 2,9,12,15,22-Pentaazatricosanedioic acid, 12,12',12''-(1,3,5-benzenetriyltricarbonyl)tris[8,16-dioxo-7,17-bis[[(phenylmethoxy)carbonyl]amino]-, hexakis(phenylmethyl) ester, (7S,7'S,7''S,17S,17'S,17''S)- (9CI) (CA INDEX NAME)

PAGE 1-B

PAGE 2-B

RN 192636-27-4 HCAPLUS

CN Carbamic acid, [[5-[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]-1,3-phenylene]bis[imino(2-oxo-2,1-ethanediyl)]]bis-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

RN 192636-28-5 HCAPLUS

CN Carbamic acid, [1,4,7,10-tetraazacyclododecane-1,4,7-triyltris[carbonyl-5,1,3-benzenetriylbis[imino(2-oxo-2,1-ethanediyl)]]]hexakis-, hexakis(phenylmethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-B

$$\begin{array}{c} \scriptsize 0 \\ \scriptsize \parallel \\ - \tt NH-C-O-CH_2-Ph \end{array}$$

RN 192636-29-6 HCAPLUS

CN Acetic acid, [2-oxo-2-[4,7,10-tris[3,5-bis[[[[(phenylmethoxy)carbonyl]amin o]acetyl]amino]benzoyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]- (9CI) (CA INDEX NAME)

PAGE 1-A

Ph-CH<sub>2</sub>-O-C-NH-CH<sub>2</sub>-C-NH

Ph-CH<sub>2</sub>-O-C-NH-CH<sub>2</sub>-C-NH

Ph-CH<sub>2</sub>-O-C-NH-CH<sub>2</sub>-C-NH

Ph-CH<sub>2</sub>-O-C-NH-CH<sub>2</sub>-C-NH

Ph-CH<sub>2</sub>-O-C-NH-CH<sub>2</sub>-C-NH

C-CH<sub>2</sub>-O-CH<sub>2</sub>-CO<sub>2</sub>H

PAGE 1-B

IT 1738-76-7, Benzyl glycinate p-toluenesulfonic acid salt 2899-60-7 21160-82-7 21160-83-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(cascade polymer precursor; nitrogen-containing cascade polymer transition metal complexes and their manufacture and use in pharmaceuticals and diagnostic agents)

RN 1738-76-7 HCAPLUS

CN Glycine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 1738-68-7 CMF C9 H11 N O2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 2899-60-7 HCAPLUS

CN Carbamic acid, [2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 21160-82-7 HCAPLUS

CN L-Lysine, N2,N6-bis[(phenylmethoxy)carbonyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & \\ & & & \\ & & \\ & & & \\$$

RN 21160-83-8 HCAPLUS

CN Carbamic acid, [(1S)-1-[[(2,5-dioxo-1-pyrrolidinyl)oxy]carbonyl]-1,5-pentanediyl]bis-, bis(phenylmethyl) ester (9CI) (CA INDEX NAME)

IT 192635-88-4P 192636-07-0P 192636-30-9P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP

(Preparation); RACT (Reactant or reagent)

(complexing cascade polymer precursor; nitrogen-containing cascade polymer transition metal complexes and their manufacture and use in pharmaceuticals and diagnostic agents)

RN 192635-88-4 HCAPLUS

CN Acetic acid, [2-oxo-2-[4,7,10-tris[1-oxo-2,6-bis[[(phenylmethoxy)carbonyl] amino]hexyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]-, 4-nitrophenyl ester, [2S-[1(R\*),1(R\*),2R\*]]-, polymer with N,N,N',N',N'',N''-hexakis(2-aminoethyl)-1,3,5-benzenetricarboxamide hydrobromide (9CI) (CA INDEX NAME)

CM 1

CRN 192635-87-3 CMF C21 H39 N9 O3 . x Br H

•x HBr

CM 2

CRN 192635-86-2 CMF C84 H99 N11 O21

PAGE 1-A

PAGE 1-B

\_\_\_ Ph

NO<sub>2</sub>

RN 192636-07-0 HCAPLUS

CN Acetic acid, [2-oxo-2-[4,7,10-tris[[[(phenylmethoxy)carbonyl]amino]acetyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]-, polymer with (all-S)-N,N,N',N'',N''-hexakis[2-[(2,6-diamino-1-oxohexyl)amino]ethyl]-1,3,5-benzenetricarboxamide hydrobromide (9CI) (CA INDEX NAME)

CM 1

CRN 192636-06-9 CMF C57 H111 N21 O9 . x Br H Absolute stereochemistry.

PAGE 1-B

RN

192636-30-9 HCAPLUS
Acetic acid, [2-oxo-2-[4,7,10-tris[3,5-bis[[[[(phenylmethoxy)carbonyl]amin CN o]acetyl]amino]benzoyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]-, polymer with N,N,N',N'',N''-hexakis(2-aminoethyl)-1,3,5-benzenetricarboxamide hydrobromide (9CI) (CA INDEX NAME)

CM 1

CRN 192636-29-6 CMF C93 H96 N16 O25

PAGE 1-B

CM 2

CRN 192635-87-3 CMF C21 H39 N9 O3 . x Br H

#### •x HBr

17 192635-93-1DP, gadolinium complexes 192636-01-4DP, gadolinium complexes 192636-31-0DP, gadolinium complexes

RL: IMF (Industrial manufacture); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(nitrogen-containing cascade polymer transition metal complexes and their manufacture and use in pharmaceuticals and diagnostic agents)

RN 192635-93-1 HCAPLUS

1,4,7,10-Tetraazacyclododecane-1,4,7-triacetic acid, 10-[2-[(carboxymethyl)amino]-2-oxoethyl]-, 1,4,7-tris(1,1-dimethylethyl) ester, polymer with N,N,N',N',N'',N''-hexakis(2-aminoethyl)-1,3,5-benzenetricarboxamide hydrobromide and [2S-[1(R\*),1(R\*),2R\*]]-4-nitrophenyl [2-oxo-2-[4,7,10-tris[1-oxo-2,6-bis[[(phenylmethoxy)carbonyl]amino]hexyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]acetate (9CI) (CA INDEX NAME)

CM 1

CN

CRN 192635-92-0

CMF C30 H55 N5 O9

CM 2

CRN 192635-87-3 CMF C21 H39 N9 O3 . x Br H

•x HBr

CM 3

CRN 192635-86-2 CMF C84 H99 N11 O21

Ö

PAGE 1-B

\_\_\_ Ph

RN 192636-01-4 HCAPLUS

CN Sodium(1+), [tris(1,1-dimethylethyl) 10-[1-methyl-2-[[2-(4-nitrophenoxy)-2-oxoethyl]amino]-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triacetate-kN1,kN4,kN7,kN10]-, bromide, polymer with N,N,N',N',N'',N''-hexakis(2-aminoethyl)-1,3,5-benzenetricarboxamide hydrobromide and 4-nitrophenyl [2-oxo-2-[4,7,10-tris[(2S)-1-oxo-2,6-bis[[(phenylmethoxy)carbonyl]amino]hexyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]acetate (9CI) (CA INDEX NAME)

CM 1

CRN 192636-00-3

CMF C37 H60 N6 Na O11 . Br

CCI CCS

● Br-

CM 2

CRN 192635-87-3 CMF C21 H39 N9 O3 . x Br H

•x HBr

CM 3

CRN 192635-86-2 CMF C84 H99 N11 O21

PAGE 1-B

\_\_\_ Ph

RN 192636-31-0 HCAPLUS

CN Sodium(1+), [tris(1,1-dimethylethyl) 10-[1-methyl-2-[[2-(4-nitrophenoxy)-2-oxoethyl]amino]-2-oxoethyl]-1,4,7,10-tetraazacyclododecane-1,4,7-triacetate-kN1,kN4,kN7,kN10]-, bromide, polymer with N,N,N',N',N'',N''-hexakis(2-aminoethyl)-1,3,5-benzenetricarboxamide hydrobromide and [2-oxo-2-[4,7,10-tris[3,5-bis[[[[(phenylmethoxy)carbonyl]amino]acetyl]amino]benzoyl]-1,4,7,10-tetraazacyclododec-1-yl]ethoxy]acetic acid (9CI) (CA INDEX NAME)

CM 1

CRN 192636-29-6 CMF C93 H96 N16 O25

PAGE 1-A

PAGE 1-B

CM 2

CRN 192636-00-3

CMF C37 H60 N6 Na O11 . Br

CCI CCS

● Br -

CM 3

CRN 192635-87-3

CMF C21 H39 N9 O3 . x Br H

•x HBr

L59 ANSWER 13 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:499124 HCAPLUS

DOCUMENT NUMBER: 127:170662

TITLE: Perfluoroalkyl-containing metal complexes and their

use in NMR diagnostics

INVENTOR(S): Platzek, Johannes; Niedballa, Ulrich; Raduchel, Bernd;

Schlecker, Wolfgang; Weinmann, Hanns-joachim; Frenzel,

Thomas; Misselwitz, Bernd; Ebert, Wolfgang

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: PCT Int. Appl., 157 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE

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WO 9726017
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                                                                       19970116 <--
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                                  19971120
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             UZ, VN
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                                               WO 1997-EP209
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                                                                   A3 19991108
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                                                                A3 20020718
                                               US 2002-197421
OTHER SOURCE(S):
                          MARPAT 127:170662
     Gd and other lanthanide and MN complexes of perfluoroalkyl-substituted
AB
     ligands of tetraazacyclododecane and polyaminoalkanes were prepared and used
     in diagnostics and therapy. The compds. according to the invention to the
     invention are particularly suited for use as in vivo contrast agents in
     nuclear spin resonance tomog. (MRT). They can be preferably used as blood
     pool agents and contrast agents for lymphog.
IT
     107-15-3, 1,2-Ethanediamine, reactions 1138-80-3,
     Benzyloxycarbonylglycine 1738-76-7
     RL: RCT (Reactant); RACT (Reactant or reagent)
        (for preparation of transition metal perfluoroalkyl-substituted
        tetraazacyclododecanes and polyaminoalkanes)
RN
     107-15-3 HCAPLUS
CN
     1,2-Ethanediamine (9CI) (CA INDEX NAME)
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 $H_2N-CH_2-CH_2-NH_2$ 

RN 1138-80-3 HCAPLUS CN Glycine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

RN 1738-76-7 HCAPLUS

CN Glycine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 1738-68-7 CMF C9 H11 N O2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

IT 51740-38-6P 193529-69-0P 193530-01-7P

193530-05-1P 193530-10-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(for preparation of transition metal perfluoroalkyl-substituted tetraazacyclododecanes and polyaminoalkanes)

RN 51740-38-6 HCAPLUS

CN 1-Octanol, 3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluoro-, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

RN 193529-69-0 HCAPLUS

CN Glycine, N-(1-carboxy-3,3,4,4,5,5,6,6,7,7,8,8,8-tridecafluorooctyl)-N[(phenylmethoxy)carbonyl]glycylglycyl- (9CI) (CA INDEX NAME)

RN 193530-01-7 HCAPLUS

CN 11-Oxa-2,5,8-triazaheneicosanoic acid, 14,14,15,15,16,16,17,17,18,18,19,19,20,20,21,21,21-heptadecafluoro-4,9-dioxo-, phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-B

 $-CH_2-Ph$ 

RN 193530-05-1 HCAPLUS

CN Carbamic acid, [2-[(3,3,4,4,5,5,6,6,7,7,8,8,9,9,10,10,10-heptadecafluorodecyl)amino]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 193530-10-8 HCAPLUS

CN Carbamic acid, [2-[4-[(heptadecafluorooctyl)sulfonyl]-1-piperazinyl]-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

$$C - CH_2 - NH - C - O - CH_2 - Ph$$
 $C - CH_2 - NH - C - O - CH_2 - Ph$ 
 $C - CH_2 - NH - C - O - CH_2 - Ph$ 

L59 ANSWER 14 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:132769 HCAPLUS

DOCUMENT NUMBER: 126:144301

TITLE: Process for preparing substituted polyazamacrocycles

and their manganese complexes

INVENTOR(S): Lennon, Patrick J.; Henke, Susan L.; Aston, Karl W. PATENT ASSIGNEE(S): Monsanto Co., USA; Lennon, Patrick J.; Henke, Susan

L.; Aston, Karl W.

SOURCE: PCT Int. Appl., 74 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.		APPLICATION NO.	DATE
WO 9640658	A1 19961219	WO 1996-US7553	19960530 <
W: AL, AM, AT,	AU, AZ, BB, BG, BR	R, BY, CA, CH, CN, CZ,	DE, DK, EE,
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LU, LV, MD,	MG, MK, MN, MW, MX	I, NO, NZ, PL, PT, RO,	RU, SD, SE,
SG, SI			
RW: KE, LS, MW,	SD, SZ, UG, AT, BE	E, CH, DE, DK, ES, FI,	FR, GB, GR,
IE, IT, LU,	MC, NL, PT, SE, BF	r, BJ, CF, CG, CI, CM,	GA, GN
CA 2224088	AA 19961219	CA 1996-2224088	19960530 <
AU 9659283	A1 19961230	AU 1996-59283	19960530 <
EP 830351	A1 19980325	EP 1996-916578	19960530 <
R: AT, BE, CH,	DE, DK, ES, FR, GB	B, GR, IT, LI, LU, NL,	SE, PT, IE, FI
JP 11507621	T2 19990706	JP 1996-500694	19960530 <
US 5721361	A 19980224	US 1996-665070	19960611 <
PRIORITY APPLN. INFO.:		US 1995-486434	A 19950607
		WO 1996-US7553	W 19960530
OTHER SOURCE(S):	CASREACT 126:14430	1; MARPAT 126:144301	

AB A process for preparing a substituted polyazamacrocycle, e.g., I (R1-R12 = H, alkyl, alkenyl, alkynyl, cycloalkyl, cycloalkenyl, heterocyclyl, aryl, etc., or selected pairs of Rn, e.g., R1R2 = O or S, etc.; A, B, C = H,

Ι

alkyl, aryl, aralkyl, cycloalkyl, organooxy, carboxylate, amide, etc.) is provided which comprises contacting a diamine R17NHCR13R14CR15R16NHR18 (R17-R18 represent a variety of acyclic or cyclic groups), or a triamine and a dicarboxylic acid or ester or anhydride thereof in the presence of a suitable base and a suitable solvent to produce the substituted polyazamacrocycle provided that when an ester of said dicarboxylic acid was used, said suitable base is optional, and when said dicarboxylic acid or an anhydride of said dicarboxylic acid was used, the reaction mixture further comprises a suitable coupling agent. The polyazamacrocycles may then be reduced by a reducing agent selected from the group consisting of aluminum hydrides and boron hydrides. The reduced substituted polyazamacrocycles are then reacted under essentially anhydrous and anaerobic conditions to produce their Mn complexes. Thus, addition of diphenylphosphoryl azide to a DMF solution of D,L-2,3-diaminobutane dihydrochloride, 3,6,9-tris(p-toluenesulfonyl)-3,6,9-triazaundecanedioic acid, and Et3N afforded after workup, racemic trans-5,6-dimethyl-3,8-dioxo-1,10,13-tris(p-toluenesulfonyl)-1,4,7,10,13-pentaazacyclopentadecane in 59% yield. Reaction of the product with LiAlH4 in THF afforded D,L-trans-2,3-dimethyl-1,4,7,10,13-pentaazacyclopentadecane (26.1% yield), which reacted with MnCl2 in anhydrous MeOH to yield the Mn(II) complex in 72% This complex and two other manganese(II) complexes of 15-membered pentaazamacrocyclic ligands are effective catalysts for the dismutation of superoxide (data given).

IT 107-15-3, 1,2-Ethanediamine, reactions 1080-44-0,
 N-p-Toluenesulfonylglycine 110345-42-1, 3,6,9-Tris(p toluenesulfonyl)-3,6,9-triazaundecanedioic acid 174291-96-4,
 N-p-Toluenesulfonyl-(1R,2R)-diaminocyclohexane
 RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of substituted polyazamacrocycles and their manganese complexes)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

 $H_2N-CH_2-CH_2-NH_2$ 

RN 1080-44-0 HCAPLUS CN Glycine, N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 110345-42-1 HCAPLUS

CN Glycine, N,N'-[[[(4-methylphenyl)sulfonyl]imino]di-2,1-ethanediyl]bis[N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

RN 174291-96-4 HCAPLUS

CN Benzenesulfonamide, N-[(1R,2R)-2-aminocyclohexyl]-4-methyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 186518-83-2P 186518-84-3P 186518-85-4P

186518-86-5P 186518-87-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation of substituted polyazamacrocycles and their manganese complexes)

RN 186518-83-2 HCAPLUS

CN D-Alanine, N-[(1R,2R)-2-[[(4-methylphenyl)sulfonyl]amino]cyclohexyl]-N[(phenylmethoxy)carbonyl]-, ethyl ester (9CI) (CA INDEX NAME)

RN 186518-84-3 HCAPLUS

CN D-Alanine, N-[(1R,2R)-2-[[(4-methylphenyl)sulfonyl]amino]cyclohexyl]-N[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 186518-85-4 HCAPLUS

CN D-Alanine, N-[(1R,2R)-2-[[(4-methylphenyl)sulfonyl]amino]cyclohexyl]-N[(phenylmethoxy)carbonyl]-D-alanyl-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 186518-86-5 HCAPLUS

CN D-Alanine, N-[(1R,2R)-2-[(2-methoxy-2-oxoethyl)][(4methylphenyl)sulfonyl]amino]cyclohexyl]-N-[(phenylmethoxy)carbonyl]-Dalanyl-, methyl ester (9CI) (CA INDEX NAME)

RN 186518-87-6 HCAPLUS

CN D-Alanine, N-[(1R,2R)-2-[(carboxymethyl)[(4-methylphenyl)sulfonyl]amino]cy clohexyl]-N-[(phenylmethoxy)carbonyl]-D-alanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L59 ANSWER 15 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:597905 HCAPLUS

DOCUMENT NUMBER: 125:301557

TITLE: Enzymic peptide synthesis in organic media. Synthesis

of CCK-8 dipeptide fragments

AUTHOR(S): Calvet, Silvia; Torres, Josep Lluis; Clapes, Pere

CORPORATE SOURCE: Unit Protein Chemistry Biochemistry, Centro

Investigacion Desarrollo-CSIC, Barcelona, 08034, Spain

SOURCE: Biocatalysis and Biotransformation (1996),

13(4), 201-216

CODEN: BOBOEQ; ISSN: 1024-2422

PUBLISHER: Harwood
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The enzymic synthesis of the seven consecutive dipeptide fragments of the cholecystokinin C-terminal octapeptide (CCK-8) in organic media is reported. The influence of the reaction medium composition, the protease, and the structure of N- $\alpha$  and C- $\alpha$  protecting groups of both carboxyl and amino components was evaluated.  $\alpha$ -Chymotryspin, papain and thermolysin adsorbed on Celite were used as catalysts, under thermodn. and kinetic control. Acetyl, benzyloxycarbonyl, tert-butyloxycarbonyl and fluoren-9-ylmethoxycarbonyl amino acid carboxamidomethyl, Me and allyl esters were assayed as carboxy components. Amino acid amide and ester

derivs. were employed as nucleophiles with a preference for the latter, since the dipeptide product obtained could be used directly, without any further chemical modification, as an acyl donor in subsequent coupling steps. All dipeptides selected were successfully synthesized, using the optimal combination of protecting groups, reaction media and enzyme different for each coupling reaction. The information gained with this study should be instrumental in designing an optimal strategy for the total enzymic synthesis of CCK-8.

Absolute stereochemistry.

(CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 29738-86-1 HCAPLUS

CN L-Tryptophanamide, N-[(phenylmethoxy)carbonyl]glycyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 53880-82-3 HCAPLUS

CN L-Tryptophan, N-[N-[(phenylmethoxy)carbonyl]glycyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 111610-57-2 HCAPLUS

CN L-Methioninamide, N-[(phenylmethoxy)carbonyl]-L-tyrosyl- (9CI) (CA INDEX NAME)

RN 159555-58-5 HCAPLUS

CN L-Tyrosine, N-[(phenylmethoxy)carbonyl]-L- $\alpha$ -aspartyl-, 2-methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 182819-08-5 HCAPLUS

Absolute stereochemistry.

RN 182819-10-9 HCAPLUS

CN L-Tyrosine, N-[N-[(phenylmethoxy)carbonyl]-L- $\alpha$ -aspartyl]-, 1-ethyl ester (9CI) (CA INDEX NAME)

RN 182819-14-3 HCAPLUS

CN L-Tyrosine, N-[N-[(phenylmethoxy)carbonyl]-L- $\alpha$ -aspartyl]-, 4-[(acetylamino)methyl] 1-methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 182819-22-3 HCAPLUS

CN Glycinamide, N-[(phenylmethoxy)carbonyl]-L-methionyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 182819-23-4 HCAPLUS

182819-27-8 HCAPLUS RN

L-Methionine, N-[N-[(phenylmethoxy)carbonyl]-L-tryptophyl]-, 2-propenyl CNester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN182819-28-9 HCAPLUS

CN L-Phenylalaninamide, N-[(phenylmethoxy)carbonyl]-L- $\alpha$ -aspartyl-, 2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

ΙT 1138-80-3 1152-61-0 1164-16-5

1668-10-6, Glycine amide hydrochloride 4668-42-2

5545-52-8 7432-21-5 53587-11-4, Tyrosine

benzyl ester tosylate 99793-10-9 127949-86-4

181135-42-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of cholecystokinin dipeptide fragments by enzymic couplings in organic media) 1138-80-3 HCAPLUS

RN

CN Glycine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

RN 1152-61-0 HCAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 1164-16-5 HCAPLUS

CN L-Tyrosine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 1668-10-6 HCAPLUS

CN Acetamide, 2-amino-, monohydrochloride (9CI) (CA INDEX NAME)

### HCl

RN 4668-42-2 HCAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, 1-methyl ester (9CI) (CA INDEX NAME)

RN 5545-52-8 HCAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, 4-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 7432-21-5 HCAPLUS

CN L-Tryptophan, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 53587-11-4 HCAPLUS

CN L-Tyrosine, phenylmethyl ester, 4-methylbenzenesulfonate (salt) (9CI) (CA INDEX NAME)

CM 1

CRN 42406-77-9

CMF C16 H17 N O3

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 99793-10-9 HCAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, 4-(2-propenyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2C$$
 $O$ 
 $S$ 
 $CO_2H$ 
 $O$ 
 $Ph$ 

RN 127949-86-4 HCAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, di-2-propenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 181135-42-2 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]-, (acetylamino)methyl ester (9CI) (CA INDEX NAME)

IT 56762-93-7P 63327-57-1P 182818-96-8P
RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(preparation of cholecystokinin dipeptide fragments by enzymic couplings in organic media)

RN 56762-93-7 HCAPLUS

CN L-Methionine, N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 63327-57-1 HCAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, 4-(1,1-dimethylethyl)
1-methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 182818-96-8 HCAPLUS

CN L-Aspartic acid, N-[(phenylmethoxy)carbonyl]-, bis[(acetylamino)methyl] ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L59 ANSWER 16 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:214774 HCAPLUS

DOCUMENT NUMBER: 124:261760

TITLE: Preparation of sulfonamide ligands and their

radioactive metal complexes and conjugates for

radiodiagnosis and therapy.

INVENTOR(S): Platzek, Johannes; Raduechel, Bernd; Kramp, Wolfgang;

Dinkelborg, Ludger

PATENT ASSIGNEE(S): Schering A.-G., Germany

SOURCE: Ger. Offen., 33 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATE	NT NO.			KINI	DATE	APPLICATION NO.		DATE	
	DE 44	425781			<b>A1</b>	19960118	DE 1994-4425781		19940714	<
	CA 2	194561			AA	19960201	CA 1995-2194561		19950622	<
	WO 96	602500			A1	19960201	WO 1995-EP2404		19950622	<
	Ţ	W: AU,	CA,	CN,	HU,	JP, KR, NO,	NZ, US			
	I	RW: AT,	BE,	CH,	DE,	DK, ES, FR,	GB, GR, IE, IT, LU,	MC, N	L, PT, SE	
	AU 95	528865			A1	19960216	AU 1995-28865		19950622	<
	AU 69	98824			B2	19981105				
	EP 7	70063			A1	19970502	EP 1995-924304		19950622	<
	I	R: AT,	BE,	CH,	DE,	DK, ES, FR,	GB, GR, IE, IT, LI,	LU, M	C, NL, PT	, SE
	CN 13	152914			Α	19970625	CN 1995-194028		19950622	<
	HU 76	6806			A2	19971128	HU 1997-101		19950622	<
	JP 10	0502648			T2	19980310	JP 1995-504625		19950622	<
	ZA 95	505896			Α	19960219	ZA 1995-5896		19950714	<
	NO 9'	700140			Α	19970313	NO 1997-140		19970113	<
P	RIORITY A	APPLN.	INFO	. :			DE 1994-4425781	Α	19940714	
							WO 1995-EP2404	W	19950622	

OTHER SOURCE(S): MARPAT 124:261760

- R2SO2NX1CHR1V1NX2V2 (CH2) pV3NX3V4 (CH2) nCH (SR3) (CH2) mR4 [V1-V4 = CO, CH(CO2H), CH2; X1 = H, (substituted) alkyl, radioactive metal ion of atomic number 43, 45, 75, 82, 83; X2, X3 = H, radioactive metal as above; n, m, p = 0, 1; m + n = 1; R1 = CO2H, UZ; U = bond, , alkylene, etc.; Z = H, amino acid, peptide, oligonucleotide, or steroid residue, etc.; R2 = (substituted) alkyl, aralkyl;R3 = H, metal ion as above, acyl, p-methoxybenzyl, ethoxyethyl, protecting group, 3,4-methylenedioxyphenyl, etc.; R4 = H, CO2H, UZ; with provisos], were prepared as diagnostic and therapeutic agents (no data). Thus, Z-Tyr-OMe in DMF was treated with KOCMe3 and 1-hexyl iodide to give 44% O-hexyl product, which was hydrogenolyzed to the N-deprotected derivative (97%). The free amine was N-tosylated (60%) and the product was stirred with ethylenediamine to give the corresponding 2-aminoethyl amide (42%). This was treated with 2-(acetylmercapto) succinic anhydride to give 31% N-p-toluenesulfonyl-2-(4hexyloxybenzyl)-2-aminoacetic acid N-[2-N-(3-carboxy-2-acetylmercapto-1oxopropyl)]aminoethylamide.
- 1T 98-59-9, p-Toluenesulfonyl chloride 107-15-3,
  1,2-Ethanediamine, reactions 1182-65-6, Cholesteryl tosylate
  13512-31-7
  - RL: RCT (Reactant); RACT (Reactant or reagent)

(preparation of sulfonamide ligands and their radioactive metal complexes and conjugates for radiodiagnosis and therapy)

RN 98-59-9 HCAPLUS

CN Benzenesulfonyl chloride, 4-methyl- (9CI) (CA INDEX NAME)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

 $H_2N-CH_2-CH_2-NH_2$ 

RN 1182-65-6 HCAPLUS

CN Cholest-5-en-3-ol  $(3\beta)$ -, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 13512-31-7 HCAPLUS

CN L-Tyrosine, N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 175214-16-1P 175214-20-7P 175214-24-1P

175214-51-4P 175214-55-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(preparation of sulfonamide ligands and their radioactive metal complexes and conjugates for radiodiagnosis and therapy)

RN 175214-16-1 HCAPLUS

CN L-Tyrosine, O-[[4-(hexyloxy)phenyl]methyl]-N-[(phenylmethoxy)carbonyl]-,
methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} O \\ O \\ O \\ O \end{array}$$

RN 175214-20-7 HCAPLUS

CN L-Tyrosine, O-[(4-methoxyphenyl)methyl]-N-[(phenylmethoxy)carbonyl]-,
 methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175214-24-1 HCAPLUS

CN L-Tyrosine, O-[[4-(dodecyloxy)phenyl]methyl]-N-[(phenylmethoxy)carbonyl]-,
 methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c} \text{O} \\ \text{$$

RN 175214-51-4 HCAPLUS

CN L-Tyrosine, O-[2-(1,1-dimethylethoxy)-2-oxoethyl]-N[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 175214-55-8 HCAPLUS

CN Benzeneacetic acid,  $4-[[2-[2-[[(3\beta)-cholest-5-en-3-yl]oxy]ethoxy]methyl]-\alpha-[[(phenylmethoxy)carbonyl]amino]-, methyl ester, (S)- (9CI) (CA INDEX NAME)$ 

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

L59 ANSWER 17 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:773016 HCAPLUS

DOCUMENT NUMBER: 124:30423

TITLE: Conformationally constrained peptide mimics as HIV

protease inhibitors

INVENTOR(S): Callahan, James F.; Huffman, William F.; Moore,

Michael L.; Newlander, Kenneth A.

PATENT ASSIGNEE(S): SmithKline Beecham Corp., USA

SOURCE: U.S., 29 pp. Cont.-in-part of U.S. Ser. No. 620, 978,

abandoned.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PAT	CENT	NO.			KIN	D	DATE			API	PLICA	TION	NO.		DATE	
						-						<b>-</b>				
US	5438	118			Α		1995	0801		US	1993	-661	36		19930726	<
WO	9209	297			A1		1992	0611		WO	1991	-US8	850		19911125	<
	W:	AU,	CA,	JP,	KR,	US										
	DLT.	7 ID	חת	CII	DE	DIZ	DO.	TI D	an	ar				O.D.		

RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LU, NL, SE

PRIORITY APPLN. INFO.: US 1990-620978 B2 19901130

WO 1991-US8850 W 19911125

OTHER SOURCE(S): MARPAT 124:30423

GI

$$\begin{array}{c|c}
R^1 \\
R^2 \\
D - W & V - X
\end{array}$$

AB Peptide mimics I in which D is A' or AB(Q)a(G)bNHCHR3; X is CHR4CO(Y)c(E)dZ or CHR4Z; V and W are each independently N or C; one of --

indicated bonds is a double bond and the other is a single bond or, when W is N, -- both are single bonds; R is hydrogen or OH, or when W is N, R is :O; R1 is C1-6 alkyl, (CH2)nAr, (CH2)n Het, (CH2)nCONHR', (CH2)nOR' or (CH2)nSR'; R2 is: (a) 2H, when V is N; (b) OH, OR', :CHR' or NHR', when (c) :0, when W and V are both N; A' is hydrogen, C1-6 alkyl, benzyl, halobenzyl, dihalobenzyl or tosyl; A is hydrogen or an amino protecting group; B is a D or L amino acid or is a covalent bond; Q is a D or L amino acid selected for Ser, Thr, Asp, His, Cys, Arg and Ala; G is Glx, Asx, Ala,  $\beta$ -Ala, Arg, Gly, Ile, Leu, Lys, Ser, Thr, Val, Met or His; Y and E are each independently a D or L amino acid; a, b, c and d are each independently 0 or 1; Z = e.g., H, (CH2)nOR'; R3 and R4 are each independently, e.g., hydrogen, C1-6 alkyl, (CH2)nHet, (CH2)nAr; R' is hydrogen, C1-4 alkyl or benzyl; n is 0 to 3; p is 1 to 3; Het is indolyl or imidazolyl, or pyridyl or thienyl optionally substituted by one or two C1-4 alkyl, OR' or SR'; and Ar is Ph optionally substituted by one or two C1-4 alkyl, OR', NO2, NH2, halogen, CF3 or SR'; or a pharmaceutically acceptable salt thereof, having a constrained peptide backbone conformation, are HIV protease inhibitors. Thus, e.g., 2-[3-benzyl-5-(1-alanylamino-ethyl)-2,3,6,7-tetrahydro-1H-2-oxo-azepin-1yl]-1-oxopropyl-valinyl-valine Me ester II, prepared via cyclization of an intermediate aminohex-3-enoic ester III (preparation given), exhibited inhibition of HIV protease at 100 µM. 2-[3-Benzyl-5-(1-alanylaminoethyl)-2,3,6,7-tetrahydro-1H-azepin-1-yl]-1-oxopropyl-valinyl-valine Me ester, similarly prepared, exhibited inhibition at 0.6  $\mu$ M. Pharmaceutical formulations were given.

IT 143590-11-8P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(conformationally constrained peptide mimics as HIV protease inhibitors)

RN 143590-11-8 HCAPLUS

CN 1H-1,4-Diazepine-1-acetic acid, hexahydro-α-methyl-5,7-dioxo-4-[1[[1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]ethyl]-6(phenylmethyl)-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

IT 1142-20-7 42854-62-6, L-Alanine benzyl ester ptoluenesulfonic acid salt

RL: RCT (Reactant); RACT (Reactant or reagent)
(conformationally constrained peptide mimics as HIV protease

inhibitors)

RN 1142-20-7 HCAPLUS

CN L-Alanine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 42854-62-6 HCAPLUS

CN L-Alanine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 17831-01-5

CMF C10 H13 N O2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

IT 50300-96-4P 143590-08-3P 143590-09-4P

143937-94-4P 143937-95-5P 143937-96-6P

143937-99-9P 143938-03-8P 143938-09-4P

144014-06-2P 171243-69-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(conformationally constrained peptide mimics as HIV protease inhibitors)

RN 50300-96-4 HCAPLUS

Absolute stereochemistry. Rotation (-).

RN 143590-08-3 HCAPLUS

CN L-Alanine, N-[2-[(2-amino-1-methyl-2-oxoethyl)amino]ethyl]-N[(phenylmethoxy)carbonyl]-, 1,1-dimethylethyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 143590-09-4 HCAPLUS

CN Benzenepropanoic acid,  $\alpha$ -[[(2-amino-1-methyl-2-oxoethyl)[2-[[2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl][(phenylmethoxy)carbonyl]amino]ethyl]a mino]carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 143937-94-4 HCAPLUS

RN 143937-95-5 HCAPLUS

Absolute stereochemistry.

RN 143937-96-6 HCAPLUS

CN L-Phenylalanine, N-[2-[[2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl][(phenylmethoxy)carbonyl]amino]ethyl]-, methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 143937-99-9 HCAPLUS

CN L-Phenylalanine, N-[2-[[2-(1,1-dimethylethoxy)-1-methyl-2-oxoethyl][(phenylmethoxy)carbonyl]amino]ethyl]-N-[3-oxo-3-(phenylmethoxy)-2-(phenylmethyl)propyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 143938-03-8 HCAPLUS

CN L-Valine, N-[N-[2-[hexahydro-5-oxo-4-[1-[[1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]ethyl]-6-(phenylmethyl)-1H- 1,4-diazepin-1-yl]-1-oxo-3-phenylpropyl]-L-valyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 143938-09-4 HCAPLUS

CN L-Alanine, N-[(phenylmethoxy)carbonyl]-N-2-propenyl-, 1,1-dimethylethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144014-06-2 HCAPLUS

CN L-Valine, N-[N-[1-0x0-2-[2,3,6,7-tetrahydro-2-0x0-5-[1-[[1-0x0-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]ethyl]-3-(phenylmethyl)-1Hazepin-1-yl]propyl]-L-valyl]-, methyl ester (9CI) (CA INDEX NAME)

171243-69-9 HCAPLUS RN

CN L-Alanine, N-(carboxymethyl)-N-[(phenylmethoxy)carbonyl]-, 1-(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L59 ANSWER 18 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1995:593387 HCAPLUS

DOCUMENT NUMBER: 123:340941

TITLE: Zinc complexes of amino acids and peptides. 5. Zinc

complexes of histidine-containing di- and tripeptides

AUTHOR (S): Foerster, Martin; Vahrenkamp, Heinrich

CORPORATE SOURCE: Institut fuer Anorganische und Analytische Chemie, Universitaet Freiburg, Freiburg, D-79104, Germany

SOURCE: Chemische Berichte (1995), 128(6), 541-50

CODEN: CHBEAM; ISSN: 0009-2940

PUBLISHER: VCH DOCUMENT TYPE: Journal English LANGUAGE:

Nine dipeptides and one tripeptide containing histidine were converted into anal. pure zinc complexes. Four different compns. were observed The peptides used as or converted into the monoacids LH (HisGly, GlyHis, HisPhe, HisHis) form the compds. ZnL2 (11a, 12-14) and alternatively (HisGly, HisGlyGly) the compds. ZnL(BF4). The peptides used as amides (HisGlyNH2, HisMetNH2) act as neutral ligands in the compds. ZnL2(ClO4)2

(15, 16). The three remaining peptides (HisAsp, AlaHis, β-AlaHis) behave like diprotonic acids LH2 forming the compds. ZnL. Spectra and solubilities indicate that complexes 11a, 13, 15, and 16 are mononuclear containing two chelating peptides bound by their amino and imidazole nitrogen atoms. All other complexes seem to be coordinated polymers in some of which the amide N and O atoms are involved in the coordination. This was proven by a structure determination for 12 in which the zinc ions are coordinated

octahedrally by two histidine N, two amino N, and two amide O atoms of four peptide residues.

IT 1668-10-6, Glycinamide hydrochloride 1738-76-7

2886-33-1 5002-64-2, Ethyl phenylalaninate tosylate

RL: RCT (Reactant); RACT (Reactant or reagent)

(zinc complexes of histidine-containing di- and tripeptides)

RN 1668-10-6 HCAPLUS

CN Acetamide, 2-amino-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 1738-76-7 HCAPLUS

CN Glycine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 1738-68-7 CMF C9 H11 N O2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 2886-33-1 HCAPLUS

CN L-Aspartic acid, bis(phenylmethyl) ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 2791-79-9 CMF C18 H19 N O4

Absolute stereochemistry. Rotation (+).

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 5002-64-2 HCAPLUS

CN L-Phenylalanine, ethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 3081-24-1 CMF C11 H15 N O2

Absolute stereochemistry.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

IT 31321-63-8P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(zinc complexes of histidine-containing di- and tripeptides)

RN 31321-63-8 HCAPLUS

CN L-Histidine, N-[N-[(phenylmethoxy)carbonyl]glycyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L59 ANSWER 19 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:631369 HCAPLUS

DOCUMENT NUMBER: 121:231369

TITLE: Preparation of amino acid and peptide derivatives as

cancer metastasis inhibitors

INVENTOR(S): Nishikawa, Naoyuki; Orikasa, Atsushi; Komazawa,

Hiroyuki; Kojima, Masayoshi; Saiki, Ikuo; Azuma,

Ichiro

PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan

SOURCE: PCT Int. Appl., 77 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND DATE	APPLICATION NO.	DATE
NO. 0304440	71 10031000	WO 1002 TD724	10020601
WO 9324448	A1 19931209	WO 1993-JP734	19930601 <
W: CA, US			
RW: AT, BE, CH,	DE, DK, ES, FR,	GB, GR, IE, IT, LU, MC,	NL, PT, SE
JP 06049013	A2 19940222	JP 1993-119848	19930521 <
JP 3274225	B2 20020415		
EP 644181	A1 19950322	EP 1993-910424	19930601 <
EP 644181	B1 19960904		
R: BE, CH, DE,	ES, FR, GB, IT,	LI, NL	
ES 2094542	T3 19970116	ES 1993-910424	19930601 <
PRIORITY APPLN. INFO.:		JP 1992-142607	A 19920603

JP 1993-119848

Ι

A 19930521

WO 1993-JP734

W 19930601

OTHER SOURCE(S):

MARPAT 121:231369

GΙ

AΒ An amino acid derivative represented by general formula (I), a pharmacol. acceptable salt thereof, and a cancer metastasis inhibitor containing the same, wherein L1 and L2 represent each an amino acid residue, etc.; A1 and A3 represent each C = O; A2 represents alkylene, etch.; m and n represent each an integer of 1 to 5; V represents -NHC(=NH)NH2, etc.; W represents -COOH, etc.; R1 and R2 represent each hydrogen, alkyl, etc.; R3 and R4 represent each hydrogen, etc.; and X and Y represent each -NH- or -O-, are prepared The derivative has a potent effect of inhibiting cancer metastasis with reduced activity of inhibiting platelet agglutination and anticoagulant activity. E.g., a mixture of malonic acid, H-Asp(OBz1)2 p-toluenesulfonate, H-Arg(NO2)-OBzl p-toluenesulfonate, and disiopropylamine in CHCl3 was stirred overnight to give, after deprotection, the title compound II, isolated as the hydrochloride, which at 1000 µg/mouse had inhibiting effect on B16-BL6 melonomer cells comparable to that of the known peptide H-Arg-Gly-Asp-Ser-OH.

II

IT 2886-33-1P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for cancer metastasis inhibitors)

RN 2886-33-1 HCAPLUS

CN L-Aspartic acid, bis(phenylmethyl) ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 2791-79-9 CMF C18 H19 N O4

Absolute stereochemistry. Rotation (+).

$$Ph$$
 $O$ 
 $NH_2$ 
 $O$ 
 $Ph$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

IT 107-15-3, 1,2-Ethanediamine, reactions 2791-84-6

2886-33-1, Aspartic acid dibenzyl ester p-toluenesulfonate

10342-07-1 158157-54-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of cancer metastasis inhibitors)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

 $H_2N-CH_2-CH_2-NH_2$ 

RN 2791-84-6 HCAPLUS

CM 1

CRN 2768-50-5

CMF C19 H21 N O4

Absolute stereochemistry.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 2886-33-1 HCAPLUS

CN L-Aspartic acid, bis(phenylmethyl) ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 2791-79-9 CMF C18 H19 N O4

Absolute stereochemistry. Rotation (+).

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 10342-07-1 HCAPLUS

CN L-Ornithine, N5-[imino(nitroamino)methyl]-, phenylmethyl ester, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 7672-27-7 CMF C13 H19 N5 O4

$$O_2N$$
 $NH$ 
 $NH$ 
 $O_2N$ 
 $NH$ 
 $O_2N$ 
 $NH$ 
 $O_2N$ 
 $O_3$ 
 $O_4$ 
 $O_4$ 
 $O_5$ 
 $O_4$ 
 $O_5$ 
 $O_5$ 
 $O_7$ 
 $O_7$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 158157-54-1 HCAPLUS

CN 2-Oxa-4,6,11-triazadodecan-12-oic acid, 5-imino-3-oxo-1-phenyl-10-[(phenylmethoxy)carbonyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L59 ANSWER 20 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1994:604946 HCAPLUS

DOCUMENT NUMBER:

121:204946

TITLE:

Process for the preparation of C-substituted

diethylenetriamines

INVENTOR(S):

Petrov, Orlin; Hilscher, Jean-Claude; Nickisch, Klaus;

Schmitt-Willich, Heribert; Gries, Heinz; Raduechel,

Bernd; Platzek, Johannes Schering A.-G., Germany

PATENT ASSIGNEE(S): SOURCE:

Ger. Offen., 8 pp.

CODEN: GWXXBX

DOCUMENT TYPE:

Patent

LANGUAGE:

German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.					KIN	)	DATE		APPLICATION NO.						DA	DATE			
						-											- <b></b> -		
DE	4302	289			<b>A1</b>		1994	0728		DE	1993	3 - 4 3	3022	89		19	9301	L25	<
WO	9417	033			A1		1994	0804		WO	1994	1-EI	P34			19	9401	L08	<
	W:	AU,	CA,	HU,	JP,	KR,	NO,	NZ,	US										
	RW:	AT,	BE,	CH,	DE,	DK,	ES,	FR,	GB,	GR	, IE	Ξ, 3	IT,	LU,	MC,	NL,	PT,	SE	
AU	9458	812			A1		1994	0815		AU	1994	1-58	8812			19	9401	108	<
AU	6813	73			B2		1997	0828											
EP	6804	67			A1		1995	1108		ΕP	1994	1-90	0501	3		19	9401	L08	<
ΕP	6804	67			B1		1998	0422											

## Hoffman 10\_631358

R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE HU 71742 A2 19960129 HU 1995-1877 19940108 <--JP 08504827 T2 19960528 JP 1994-516608 19940108 <--JP 3481242 **B2** 20031222 AT 165341 Ε 19980515 AT 1994-905013 19940108 <--ES 2115930 **T3** 19980701 ES 1994-905013 19940108 <--IL 108346 **A1** 19981030 IL 1994-108346 19940116 <--CN 1100411 Α 19950322 CN 1994-102662 19940124 <--CN 1055460 В 20000816 ZA 9400514 Α 19940905 ZA 1994-514 19940125 <--AA 19940804 CA 1994-2154558 CA 2154558 19940128 <--NO 9502926 Α 19950724 NO 1995-2926 19950724 <--B1 NO 305116 19990406 19970805 US 1995-495474 19951012 <--US 5654467 PRIORITY APPLN. INFO.: DE 1993-4302289 19930125 WO 1994-EP34 19940108

OTHER SOURCE(S): MARPAT 121:204946

The title compds. R4HNCH(R1)CH2NHCH(R3)CH(R2)NH2 [R1 = (CH2)m(C6H4)q(O)k(CH2)n(C6H4)1(O)rR, (CH2)m(C6H10)q(O)k(CH2)n(C6H10)1(O)rR; R = H, protecting group, (un)substituted C1-6 alkyl, etc.; k, l, q, r = 0, 1; m, n = 0-5; R2, R3 = H; R4 = amino-protective group; R2R3 = (CH2)p; p = 3, 4] are prepared, without the use of diboranes, by the condensation of aminoethyl alcs. R4HNCH(R1)CH2OH with methanesulfonyl chloride, tosyl chloride, or trifluroacetic anhydride, and the intermediate is treated with ethylenediamine H2NCH(R2)CH(R3)NH2.

IT 121778-71-0P 158043-51-7P 158043-61-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of C-substituted diethylenetriamines)

RN 121778-71-0 HCAPLUS

CN L-Tyrosine, O-methyl-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CAINDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 158043-51-7 HCAPLUS

CN L-Tyrosine, O-ethyl-N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 158043-61-9 HCAPLUS

CN Carbamic acid, [2-{(2-aminocyclohexyl)amino}-1-[(4-methoxyphenyl)methyl]-2-oxoethyl]-, phenylmethyl ester, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

H2N-CH2-CH2-NH2

RN 1161-13-3 HCAPLUS

CN L-Phenylalanine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

RN 13512-31-7 HCAPLUS

CN L-Tyrosine, N-[(phenylmethoxy)carbonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L59 ANSWER 21 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:212035 HCAPLUS

DOCUMENT NUMBER: 120:212035

TITLE: Universal standard reagents for analyzing compounds

having functional groups, method of preparing same,

and use thereof

INVENTOR(S):
Patchornik, Avraham

PATENT ASSIGNEE(S): Patchornik, Zipora, Israel

SOURCE: PCT Int. Appl., 45 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIN	D DATE	APPLICATION NO.	DATE			
WO 9401771	A1	. 19940120	WO 1993-US6980	19930714 <			
W: AT, A	, BB, BG,	BR, BY, CA,	CH, CZ, DE, DK, ES,	FI, GB, HU, JP,			
KP, KI	, KZ, LK,	LU, MG, MN,	MW, NL, NO, NZ, PL,	PT, RO, RU, SD,			
SE, SI	, UA, US,	VN					
RW: AT, BI	, CH, DE,	DK, ES, FR,	GB, GR, IE, IT, LU,	MC, NL, PT, SE,			
BF, B	, CF, CG,	CI, CM, GA,	GN, ML, MR, NE, SN,	TD, TG			
IL 102495	A1	. 19980615	IL 1992-102495	19920714 <			
AU 9347844	A1	. 19940131	AU 1993-47844	19930714 <			
EP 650595	A1	. 19950503	EP 1993-918367	19930714 <			
R: AT, BI	, CH, DE,	DK, ES, FR,	GB, GR, IE, IT, LI,	LU, MC, NL, PT, SE			
JP 08505220	Т2	19960604	JP 1993-503596	19930714 <			
US 5576216	Α	19961119	US 1995-362519	19950105 <			
PRIORITY APPLN. IN	0.:		IL 1992-102495	A 19920714			
			WO 1993-US6980	A 19930714			
OFFITTE COTTON (C)			a =				

OTHER SOURCE(S): MARPAT 120:212035

## Hoffman 10\_631358

AB A universal standard chemical reagent is described for quant. visual and spectrometric anal. of compds. having reactive functional groups, including mixts. and homologs of the compds. The reagent comprises compound Q-B-f (Q = organic moiety which can be measured quant., visually by color, spectroscopically, or fluorometrically; B = nonreactive organic bridging unit linking Q to a reactive functional group f, the bridging unit being of sufficient length or size to prevent any possible interaction of Q that might alter its spectroscopic properties even upon derivatization; f = reactive group which can react with a compound to form covalently bonded derivs.). Chlorodinitrobenzene was reacted with 3-aminopropanol in MeOH to make DNPNH(CH2)3OH (I). I enabled the prediction of the existence of self-catalytic reactions in acetylated glucose. DNPNH(CH2)3NHNH2 was used to analyze a triglyceride.

IT 98-59-9, Tosyl chloride

RL: ANT (Analyte); ANST (Analytical study)

(anal. of, spectrometric, dinitrophenylaminoethylenediamine or other compound as universal standard reagent for)

RN 98-59-9 HCAPLUS

CN Benzenesulfonyl chloride, 4-methyl- (9CI) (CA INDEX NAME)

IT 3588-57-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(coupling reaction of, with dinitrophenylamine reagent, diastereomers study in relation to)

RN 3588-57-6 HCAPLUS

CN Phenylalanine, N-[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

 $HO_2C-CH-CH_2-Ph$ 

IT 154036-19-8 154036-20-1

RL: FORM (Formation, nonpreparative)

(formation of, with dinitrophenylamine reagent, diastereomers study in relation to)

RN 154036-19-8 HCAPLUS

CN L-Valinamide, N-[(phenylmethoxy)carbonyl]-L-phenylalanyl-N-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

RN 154036-20-1 HCAPLUS

CN L-Valinamide, N-[(phenylmethoxy)carbonyl]-D-phenylalanyl-N-[2-[(2,4-dinitrophenyl)amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 107-15-3, 1,2-Ethanediamine, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of universal standard reagent for spectrometric and

visual anal. of compds. containing functional groups)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

H2N-CH2-CH2-NH2

L59 ANSWER 22 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:153723 HCAPLUS

DOCUMENT NUMBER: 120:153723

TITLE: Use of calpain inhibitors in the inhibition and

treatment of medical conditions associated with

increased calpain activity

INVENTOR(S): Eveleth, David D., Jr.; Lynch, Gary; Powers, James C.;

Bartus, Raymond T.

PATENT ASSIGNEE(S): Cortex Pharmaceuticals, Inc., USA; Georgia Tech

Research Corp.

SOURCE: PCT Int. Appl., 255 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

## Hoffman 10 631358

PAT	PATENT NO.						KIND DATE			APPLICATION NO.						DATE				
											<b>-</b> -									
WO	WO 9400095					A2 19940106			1	WO 1	993-1	US61	19930624 <							
WO	WO 9400095						1994	0317												
	W:	ΑT,	AU,	BB,	BG,	BR,	CA,	CH,	CZ,	DE,	DK,	ES,	FI,	GB,	HU,	JP,	KP,			
		KR,	ΚZ,	LK,	LU,	MG,	MN,	MW,	NL,	NO,	NZ,	PL,	PT,	RO,	RU,	SD,	SE,			
		SK,	UA,	US,	VN															
	RW:	AT,	ΒE,	CH,	DE,	DK,	ES,	FR,	GB,	GR,	ΙĒ,	IT,	LU,	MC,	NL,	PT,	SE,			
		BF,	ВJ,	CF,	CG,	CI,	CM,	GA,	GN,	ML,	MR,	NΕ,	SN,	TD,	TG					
AU	9345	449			A1		1994	0124		AU 1	993-	4544	9		1	9930	624	<		
JP 09500087						2 19970107			JP 1993-502621						1	9930	524	<		
PRIORITY APPLN. INFO.:										US 1992-903800					A2 19920624					
									,	US 1	993-	3499	6		A2 1	9930	316			
											US 1993-72609					A2 19930601				
										WO 1	993-	US61	43		A 1	9930	624			

AB Medical conditions in mammals (e.g. cardiac muscle tissue damage, cataracts, smooth muscle damage, and vasospasm) associated with increased proteolytic activity of calpain are treated by administering a pharmaceutical composition containing a calpain inhibitor in a pharmacol. effective

amount The inhibitor is a peptide keto compound, substituted heterocyclic compound, or halo ketone peptide. Also, a method of inhibiting proliferation of smooth muscle cells and thereby preventing the restenosis of a blood vessel which has undergone therapeutic angioplasty includes the administration of a calpain inhibitor to the blood vessel during or after the angioplasty. Further, methods of blocking the establishment of the tonically contracted state in smooth muscle and relaxing tonically contracted smooth muscle are disclosed. These methods involve the administration of a calpain inhibitor, thereby reducing or preventing smooth muscle contraction associated with vasospasm and bronchospasm.

IT 402-71-1, TPCK

RL: BIOL (Biological study)

(as calpain inhibitor, glutamate neurotoxicity prevention by)

RN 402-71-1 HCAPLUS

CN Benzenesulfonamide, N-[(1S)-3-chloro-2-oxo-1-(phenylmethyl)propyl]-4-methyl- (9CI) (CA INDEX NAME)

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TT 102330-03-0 102330-05-2 144231-35-6 144231-36-7 144231-38-9 144231-43-6 144231-44-7 144231-45-8 144231-46-9 144231-63-0 144231-64-1 144231-62-9 144231-68-5 144231-69-6 144231-70-9 144231-71-0 144231-72-1 144231-73-2 144231-77-6 144231-75-4 144231-79-8 144231-80-1 144231-81-2 144231-85-6
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## Hoffman 10\_631358

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144231-87-8 144231-88-9 144231-89-0
     144232-07-5 144248-87-3 144248-90-8
     144248-91-9 144248-92-0 144248-93-1
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     153370-38-8 153370-39-9 153370-40-2
     153370-41-3 153370-42-4 153370-43-5
     153370-44-6 153370-45-7 153370-46-8
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     153370-71-9 153370-72-0 153370-73-1
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     153370-77-5 153370-78-6 153370-79-7
     153370-80-0 153370-81-1 153370-82-2
     153370-83-3 153370-84-4 153370-85-5
    153370-86-6 153370-87-7 153370-88-8
    153370-89-9 153370-90-2 153370-91-3
    153370-92-4 153410-31-2
    RL: BIOL (Biological study)
        (as calpain inhibitor, heart and vascular disease treatment with)
RN
     102330-03-0 HCAPLUS
    L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-N-(3-ethoxy-1-ethyl-
CN
     2,3-dioxopropyl)- (9CI) (CA INDEX NAME)
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Absolute stereochemistry.

RN 102330-05-2 HCAPLUS
CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-L-alanyl-N-(3-ethoxy-1methyl-2,3-dioxopropyl)- (9CI) (CA INDEX NAME)

RN 144231-35-6 HCAPLUS

CN Butanoic acid, 2-oxo-3-[[1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 144231-36-7 HCAPLUS

CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-N-(3-ethoxy-1-methyl-2,3-dioxopropyl)- (9CI) (CA INDEX NAME)

RN 144231-38-9 HCAPLUS

CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-N-[1-(ethoxyoxoacetyl)butyl]- (9CI) (CA INDEX NAME)

RN 144231-43-6 HCAPLUS

CN Butanoic acid, 2-oxo-3-[[1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]am

ino]-, butyl ester (9CI) (CA INDEX NAME)

RN 144231-44-7 HCAPLUS

CN Butanoic acid, 2-oxo-3-[[1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 144231-45-8 HCAPLUS

CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-N-[1-ethyl-2,3-dioxo-3-(phenylmethoxy)propyl]- (9CI) (CA INDEX NAME)

RN 144231-46-9 HCAPLUS

CN Hexanoic acid, 3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl ]amino]-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 144231-47-0 HCAPLUS

CN Benzenebutanoic acid,  $\beta$ -[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]- $\alpha$ -oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 144231-48-1 HCAPLUS

CN Pentanoic acid, 3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]penty l]amino]-2-oxo-, ethyl ester (9CI) (CA INDEX NAME)

RN 144231-62-9 HCAPLUS

CN Benzenebutanoic acid, 4-chloro- $\beta$ -[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]- $\alpha$ -oxo-, ethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-63-0 HCAPLUS

CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]-L-leucyl-N-[(1S)-3-ethoxy-1-ethyl-2,3-dioxopropyl]- (9CI) (CA INDEX NAME)

RN 144231-64-1 HCAPLUS

CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]-L-leucyl-N-[3-ethoxy-2,3-dioxo-1-(phenylmethyl)propyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-67-4 HCAPLUS

CN Pentanoic acid, 3-[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino] pentyl]amino]-5-(methylthio)-2-oxo-, ethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-68-5 HCAPLUS

CN Benzenebutanoic acid,  $\beta$ -[[4-methyl-1-oxo-2- [[(phenylmethoxy)carbonyl]amino]pentyl]amino]- $\alpha$ -oxo-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-69-6 HCAPLUS

CN Pentanoic acid, 3-[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]

pentyl]amino]-2-oxo-, phenylmethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-70-9 HCAPLUS

CN Benzenebutanoic acid,  $\beta$ -[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]- $\alpha$ -oxo-, ( $\beta$ S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-71-0 HCAPLUS

CN Pentanoic acid, 3-[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino] pentyl]amino]-2-oxo-, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-72-1 HCAPLUS

CN Carbamic acid, [(1S)-1-[[(1S)-3-(butylamino)-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 144231-73-2 HCAPLUS

CN Carbamic acid, [(1S)-3-methyl-1-[[[(1S)-3-[(2-methylpropyl)amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]butyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-74-3 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-2,3-dioxo-1-(phenylmethyl)-3[(phenylmethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl
ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-75-4 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-2,3-dioxo-3-[(2-phenylethyl)amino]-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 144231-76-5 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-1-ethyl-3-(ethylamino)-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-77-6 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-1-ethyl-2,3-dioxo-3-(propylamino)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-78-7 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-3-(butylamino)-1-ethyl-2,3dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA
INDEX NAME)

RN 144231-79-8 HCAPLUS

Absolute stereochemistry.

RN 144231-80-1 HCAPLUS

CN Carbamic acid, [(1S)-1-[[(1S)-1-ethyl-2,3-dioxo-3-[(phenylmethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-81-2 HCAPLUS

CN Carbamic acid, [(1S)-1-[[(1S)-1-ethyl-2,3-dioxo-3-[(2phenylethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 144231-82-3 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-1-ethyl-3-[[3-(4-morpholinyl)propyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-83-4 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-1-ethyl-3-(octylamino)-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-84-5 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-1-ethyl-3-[(2-hydroxyethyl)amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 144231-85-6 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-3-[[(3,5-dimethoxyphenyl)methyl]amino]-1-ethyl-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-87-8 HCAPLUS

CN 2-Hexenoic acid, 2-hydroxy-3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]-, ethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 144231-88-9 HCAPLUS

CN 2-Butenoic acid, 2-hydroxy-3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]-4-phenyl-, ethyl ester, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 144231-89-0 HCAPLUS

CN 2-Pentenoic acid, 2-hydroxy-3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]-, ethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 144232-07-5 HCAPLUS

CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-leucyl-N-[1-(ethoxyoxoacetyl)-5-[[(phenylmethoxy)carbonyl]amino]pentyl]- (9CI) (CA INDEX NAME)

RN 144248-87-3 HCAPLUS

CN L-Prolinamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-N-(3-ethoxy-1-methyl-2,3-dioxopropyl)- (9CI) (CA INDEX NAME)

RN 144248-90-8 HCAPLUS

CN Heptanoic acid, 3-[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino] pentyl]amino]-2-oxo-, ethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144248-91-9 HCAPLUS

CN Benzenebutanoic acid,  $\beta$ -[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]- $\alpha$ -oxo-, butyl ester, ( $\beta$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144248-92-0 HCAPLUS

CN Pentanoic acid, 3-[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino] pentyl]amino]-2-oxo-, butyl ester, (3S)- (9CI) (CA INDEX NAME)

RN 144248-93-1 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-3-(ethylamino)-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144248-94-2 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-2,3-dioxo-1-(phenylmethyl)-3-(propylamino)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144248-95-3 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-1-ethyl-3-(octadecylamino)-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 144248-96-4 HCAPLUS

CN Carbamic acid, [(1S)-1-[[[(1S)-1-ethyl-2,3-dioxo-3-[(4-pyridinylmethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144863-87-6 HCAPLUS

CN 12-Oxa-2,5,9-triazatetradecanoic acid, 6-ethyl-14-hydroxy-3-(2-methylpropyl)-4,7,8-trioxo-, phenylmethyl ester, (3S,6S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-23-1 HCAPLUS

CN Carbamic acid, [1-[[[3-[(2-hydroxy-2-phenylethyl)amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-24-2 HCAPLUS

CN Carbamic acid, [1-[[[3-amino-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbon
yl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX
NAME)

Absolute stereochemistry.

RN 153370-25-3 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[(2-hydroxy-2-phenylethyl)amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-28-6 HCAPLUS

CN 2-Butenoic acid, 4-(4-chlorophenyl)-2-hydroxy-3-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Double bond geometry unknown.

RN 153370-29-7 HCAPLUS

CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]-L-leucyl-N-[1-(carboxyhydroxymethylene)propyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 153370-30-0 HCAPLUS

CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]-L-leucyl-N-[2-carboxy-2-hydroxy-1-(phenylmethyl)ethenyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

RN 153370-33-3 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-2,3-dioxo-3-[[2-(4-pyridinyl)ethyl]amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

RN 153370-34-4 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[(5-hydroxypentyl)amino]-2,3dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester,
[S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-35-5 HCAPLUS

CN 2-Oxa-5,9,12-triazatridecan-13-oic acid, 8-ethyl-3-methoxy-11-(2methylpropyl)-6,7,10-trioxo-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-36-6 HCAPLUS

CN 12-Oxa-2,5,9-triazatetradecanoic acid, 11-ethoxy-6-ethyl-3-(2-methylpropyl)-4,7,8-trioxo-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-37-7 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[(5-hydroxy-1,3,3-trimethylcyclohexyl)methyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-38-8 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-(4-hydroxyphenyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-39-9 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-(2-methoxyphenyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

RN 153370-40-2 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-(3-methoxyphenyl)ethyl]amino]-2,3dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester,
[S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-41-3 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-(4-methoxyphenyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-42-4 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-(3,5-dimethoxyphenyl)ethyl]amino]-1-ethyl-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

RN 153370-43-5 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-(4-methoxyphenyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-44-6 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-(2,4,6-trimethoxyphenyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-45-7 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-[4-(dimethylamino)phenyl]-2-hydroxyethyl]amino]-1-ethyl-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-46-8 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-(pentafluorophenyl)ethyl]amin o]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-47-9 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-[3-(trifluoromethyl)phenyl]ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-48-0 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-(3-phenoxyphenyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-49-1 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-(4-phenoxyphenyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-50-4 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-[4-(phenylmethoxy)phenyl]ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-51-5 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-[3-[3-(trifluoromethyl)phenoxy]phenyl]ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-52-6 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-[3-(3,4-dichlorophenoxy)phenyl]-2-hydroxyethyl]amino]-1-ethyl-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-53-7 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-[3,4-bis(phenylmethoxy)phenyl]-2-hydroxyethyl]amino]-1-ethyl-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-54-8 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-(1-naphthalenyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-55-9 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-hydroxy-2-(2-naphthalenyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-56-0 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-[4-(dimethylamino)phenyl]-2-hydroxyethyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-57-1 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-hydroxy-2-(pentafluorophenyl)ethyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-58-2 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-hydroxy-2-[3-(trifluoromethyl)phenyl]ethyl]amin
 o]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-,
 phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-59-3 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-hydroxy-2-(3-phenoxyphenyl)ethyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-60-6 HCAPLUS

CN Carbamic acid, [1-[{[3-[[2-hydroxy-2-(4-phenoxyphenyl)ethyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-61-7 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-hydroxy-2-[4-(phenylmethoxy)phenyl]ethyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-62-8 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-hydroxy-2-[3-[3-(trifluoromethyl)phenoxy]phenyl]ethyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-63-9 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-[3-(3,4-dichlorophenoxy)phenyl]-2-hydroxyethyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-64-0 HCAPLUS

CN Carbamic acid, [1-[[[3-[[2-[3,4-bis(phenylmethoxy)phenyl]-2-hydroxyethyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-65-1 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[(2-furanylmethyl)amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-66-2 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[(tetrahydro-2-furanyl)methyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Hoffman 10\_631358

RN 153370-67-3 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-2,3-dioxo-3-[(2-pyridinylmethyl)amino]propyl] amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-68-4 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-2,3-dioxo-3-[(3-pyridinylmethyl)amino]propyl] amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-69-5 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-2,3-dioxo-3-[[2-(2-pyridinyl)ethyl]amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

RN 153370-70-8 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[3-(1H-imidazol-1-yl)propyl]amino]-2,3dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester,
[S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-71-9 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-(4-morpholinyl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-72-0 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-2,3-dioxo-3-[[3-(2-oxo-1-pyrrolidinyl)propyl]amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Hoffman 10\_631358

RN 153370-73-1 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[2-(1H-indol-3-yl)ethyl]amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-74-2 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-2,3-dioxo-3-[(2-quinolinylmethyl)amino]propyl ]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-75-3 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[(1-isoquinolinylmethyl)amino]-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

RN 153370-76-4 HCAPLUS

CN Carbamic acid, [1-[[[3-[[3-(3,4-dihydro-1(2H)-quinolinyl)propyl]amino]-1-ethyl-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-77-5 HCAPLUS

CN Carbamic acid, [1-[[[3-[[3-(3,4-dihydro-2(1H)-isoquinolinyl)propyl]amino]1-ethyl-2,3-dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl
ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-78-6 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-2,3-dioxo-3-[[(2,3,6,7-tetrahydro-1,3,7-trimethyl-2,6-dioxo-1H-purin-8-yl)methyl]amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

RN 153370-79-7 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[(4-methyl-2-thiazolyl)methyl]amino]-2,3dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester,
[S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-80-0 HCAPLUS

CN 2,5,9,12-Tetraazaheptadecanoic acid, 6-ethyl-17-(hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl)-3-(2-methylpropyl)-4,7,8,13-tetraoxo-, phenylmethyl ester, [3aS-[3a $\alpha$ ,4 $\beta$ (3R\*,6R\*),6a $\alpha$ ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-81-1 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-3-[[(1-oxido-3-pyridinyl)methyl]amino]-2,3dioxopropyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester,
[S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

RN 153370-82-2 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-2,3-dioxo-3-[[(1,2,3,6-tetrahydro-2,6-dioxo-4-pyrimidinyl)methyl]amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-83-3 HCAPLUS

CN Carbamic acid, [1-[[[2,3-dioxo-1-(phenylmethyl)-3-[(2-pyridinylmethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-84-4 HCAPLUS

CN Carbamic acid, [3-methyl-1-[[[3-[[3-(4-morpholinyl)propyl]amino]-2,3-dioxo1-(phenylmethyl)propyl]amino]carbonyl]butyl]-, phenylmethyl ester,
[S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-85-5 HCAPLUS

CN Carbamic acid, [1-[[[2,3-dioxo-1-(phenylmethyl)-3-[(2-quinolinylmethyl)amino]propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-86-6 HCAPLUS

CN Carbamic acid, [1-[[[3-[(1-isoquinolinylmethyl)amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-87-7 HCAPLUS

CN Carbamic acid, [1-[[[3-[[3-(3,4-dihydro-1(2H)-quinolinyl)propyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-88-8 HCAPLUS

CN Carbamic acid, [1-[[[3-[[3-(3,4-dihydro-2(1H)-isoquinolinyl)propyl]amino]-2,3-dioxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-89-9 HCAPLUS

CN Carbamic acid, [1-[[[1-[[(2-hydroxy-2-phenylethyl)amino]oxoacetyl]butyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 153370-90-2 HCAPLUS

RN 153370-91-3 HCAPLUS

CN 2,5,9,12-Tetraazaheptadecanoic acid, 17-(hexahydro-2-oxo-1H-thieno[3,4-d]imidazol-4-yl)-3-(2-methylpropyl)-4,7,8,13-tetraoxo-6-(phenylmethyl)-, phenylmethyl ester, [3aS-[3a $\alpha$ ,4 $\beta$ (3R\*,6R\*),6a $\alpha$ ]]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153370-92-4 HCAPLUS

CN Carbamic acid, [3-methyl-1-[[[1-[[[3-(4-morpholinyl)propyl]amino]oxoacetyl]butyl]amino]carbonyl]butyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153410-31-2 HCAPLUS

CN Carbamic acid, [1-[[[1-ethyl-5-(1-methyl-1H-pyrrol-2-yl)-2,3-dioxopentyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

IT 26049-92-3 38104-37-9 41658-44-0

52386-46-6 116614-45-0 144249-07-0

RL: BIOL (Biological study)

(calpain and other proteinases inhibition by)

RN 26049-92-3 HCAPLUS

CN Carbamic acid, [2-[[3-chloro-2-oxo-1-(phenylmethyl)propyl]amino]-1-methyl-2-oxoethyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 38104-37-9 HCAPLUS

CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[(1S)-3-chloro-1-methyl-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 41658-44-0 HCAPLUS

CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-[(1S)-3-chloro-2-oxo-1-(phenylmethyl)propyl]- (9CI) (CA INDEX NAME)

RN 52386-46-6 HCAPLUS

CN Carbamic acid, [1-[[[3-chloro-2-oxo-1-(phenylmethyl)propyl]amino]carbonyl]-3-methylbutyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 116614-45-0 HCAPLUS

CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]-L-leucyl-N-[(1S)-3-diazo-1-[(4-hydroxyphenyl)methyl]-2-oxopropyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144249-07-0 HCAPLUS

CN Carbamic acid, [1-[[[3-chloro-2-oxo-1-(phenylmethyl)propyl]amino]carbonyl]-2-methylpropyl]-, phenylmethyl ester, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

144232-06-4P 144232-07-5P 145731-11-9P IT

153371-13-2P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP
(Preparation); RACT (Reactant or reagent)

(preparation and deprotection of, in calpain inhibitor preparation for heart and

vascular disease treatment)

RN144232-06-4 HCAPLUS

Heptanoic acid, 2-oxo-3-[[1-oxo-3-phenyl-2-[[(phenylmethoxy)carbonyl]amino CN ]propyl]amino]-7-[[(phenylmethoxy)carbonyl]amino]-, ethyl ester (9CI) INDEX NAME)

144232-07-5 HCAPLUS RN

L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-leucyl-N-[1-(ethoxyoxoacetyl)-CN 5-[[(phenylmethoxy)carbonyl]amino]pentyl]- (9CI) (CA INDEX NAME)

RN 145731-11-9 HCAPLUS

CN Heptanoic acid, 2-oxo-7-[[(phenylmethoxy)carbonyl]amino]-3-[[[[(phenylmethoxy)carbonyl]amino]acetyl]amino]-, ethyl ester (9CI) (CA INDEX NAME)

RN 153371-13-2 HCAPLUS

CN 2-Oxa-4,7,13-triazatetradecan-14-oic acid, 8-(2-ethoxy-1-hydroxy-2-oxoethylidene)-5-methyl-3,6-dioxo-1-phenyl-, phenylmethyl ester, (S)-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

IT 144231-55-0P 144231-57-2P 153371-09-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in calpain inhibitor preparation for heart and vascular disease treatment)

RN 144231-55-0 HCAPLUS

CN Benzenebutanoic acid,  $\beta$ -[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]- $\alpha$ -oxo-, ethyl ester, ( $\beta$ S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-57-2 HCAPLUS

CN Pentanoic acid, 3-[[(2S)-4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]

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pentyl]amino]-2-oxo-, ethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153371-09-6 HCAPLUS

CN 2-Butenoic acid, 2-hydroxy-3-[[1-oxo-2-[[(phenylmethoxy)carbonyl]amino]propyl]amino]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

Double bond geometry unknown.

IT 107-15-3, 1,2-Ethanediamine, reactions 1909-02-0

6401-63-4 13585-98-3 13883-42-6

16012-70-7 18921-54-5 35180-80-4

47802-55-1 144231-99-2 144232-00-8

144232-02-0 144232-08-6 144232-23-5

144249-01-4 153371-10-9 153371-11-0

153371-14-3

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in calpain inhibitor preparation for heart and vascular disease treatment)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

 $H_2N-CH_2-CH_2-NH_2$ 

RN 1909-02-0 HCAPLUS

CN L-Lysine, N6-[(phenylmethoxy)carbonyl]-N2-[N-[(phenylmethoxy)carbonyl]-L-phenylalanyl]- (9CI) (CA INDEX NAME)

RN 6401-63-4 HCAPLUS

CN L-Phenylalanine, N-[(phenylmethoxy)carbonyl]-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 13585-98-3 HCAPLUS

CN L-Alanine, N-[(phenylmethoxy)carbonyl]-L-alanyl-L-alanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 13883-42-6 HCAPLUS

CN L-Alanine, N-[(phenylmethoxy)carbonyl]-L-alanyl-L-alanyl-L-alanyl- (9CI) (CA INDEX NAME)

RN 16012-70-7 HCAPLUS

CN L-Alanine, N-[(phenylmethoxy)carbonyl]-L-alanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 18921-54-5 HCAPLUS

CN L-Norvaline, N-[N-[(phenylmethoxy)carbonyl]-L-alanyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 35180-80-4 HCAPLUS

CN L-Lysine, N6-[(phenylmethoxy)carbonyl]-N2-[N-[(phenylmethoxy)carbonyl]glyc yl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ \text{Ph} & & & \\$$

RN 47802-55-1 HCAPLUS

CN L-Phenylalanine, N-[(phenylmethoxy)carbonyl]-L-leucyl-L-leucyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144231-99-2 HCAPLUS

CN Butanoic acid, N-[(phenylmethoxy)carbonyl]-L-alanyl-L-alanyl-2-amino-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144232-00-8 HCAPLUS

CN L-Alanine, N-[1-[N-[(phenylmethoxy)carbonyl]-L-alanyl]-L-prolyl]-, compd. with N-cyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 61430-15-7 CMF C19 H25 N3 O6

CM 2

CRN 101-83-7 CMF C12 H23 N

RN 144232-02-0 HCAPLUS

CN Butanoic acid, 2-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl ]amino]-, [S-(R\*,R\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 144232-08-6 HCAPLUS

CN Lysine, N6-[(phenylmethoxy)carbonyl]-N2-[N-[N-[(phenylmethoxy)carbonyl]-L-leucyl]-L-alanyl]- (9CI) (CA INDEX NAME)

RN 144232-23-5 HCAPLUS

CN L-Phenylalanine, 4-chloro-N-[N-[(phenylmethoxy)carbonyl]-L-leucyl]- (9CI) (CA INDEX NAME)

RN 144249-01-4 HCAPLUS

CN Butanoic acid, N-[(phenylmethoxy)carbonyl]-L-leucyl-L-leucyl-L-2-amino-(9CI) (CA INDEX NAME)

RN 153371-10-9 HCAPLUS

CN L-Norvaline, N-[N-[(phenylmethoxy)carbonyl]-L-leucyl]- (9CI) (CA INDEX NAME)

RN 153371-11-0 HCAPLUS

CN Lysine, N6-[(phenylmethoxy)carbonyl]-N2-[N-[(phenylmethoxy)carbonyl]-L-alanyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 153371-14-3 HCAPLUS

CN 1,3-Dithiolane-2-carboxylic acid, 2-[1-[[4-methyl-1-oxo-2-[[(phenylmethoxy)carbonyl]amino]pentyl]amino]butyl]-, ethyl ester, [S-(R\*,S\*)]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

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ACCESSION NUMBER: 1993:495559 HCAPLUS

DOCUMENT NUMBER: 119:95559

TITLE: Preparation of benzodiazepinones as cholecystokinin

and gastrin antagonists

INVENTOR(S): Chambers, Mark S.; Fletcher, Stephen R.; Matassa,

Victor G.

PATENT ASSIGNEE(S): Merck Sharp and Dohme Ltd., UK

SOURCE: Eur. Pat. Appl., 53 pp.

CODEN: EPXXDW

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DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

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PATENT NO.	KIND	DATE	AP	PLICATION NO.	DATE		
EP 514133	A1	19921119	EP	1992-304264		19920512	<
R: CH, DE, FR,	GB, IT	, LI, NL					
CA 2068355	AA	19921115	CA	1992-2068355		19920511	<
JP 05178843	A2	19930720	JP	1992-122170		19920514	<
PRIORITY APPLN. INFO.:			GB	1991-10438	Α	19910514	
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			GB	1991-22664	A	19911025	
			GB	1992-1104	Α	19920120	

OTHER SOURCE(S): MARPAT 119:95559

GΙ

$$(R^3)_{x} \xrightarrow{R^1} \overset{O}{\underset{R^4}{0}} \overset{O}{\underset{H}{0}} \overset{O}{\underset{H}{0}} \overset{R^2}{\underset{H}{0}}$$

Title compds. I [R1 = (CH2)qR, (substituted) C1-6 alkyl, C3-7 cycloalkyl, cyclopropylmethyl, CH2CO2R5, CH2CONR6R7, CH2CHOHW(CH2)2NR6R7; R = imidazolyl, tetrazolyl, triazolyl; R5 = C1-4 alkyl; R6, R7 = H, C1-4 alkyl or NR6R7 = pyrrolidinyl, piperidinyl; q = 1-3; W = S, NH; R2 = (substituted) Ph, pyridinyl, etc.; R3 = C1-6 alkyl, halo; R4 = C3-7 cycloalkyl; x = 0-3] were prepared as cholecystokinin (CCK) and gastrin antagonists. Thus, 2-(COR)C6H4NHCOCH(NH2)NHCO2CH2Ph (R = cyclohexyl) (preparation given) was cyclized in the presence of AcONH4/HOAc to give the benzodiazepinone derivative This was N-methylated by MeI, N-deprotected, then treated with m-tolyl isocyanate to give title compound I [R1 = Me; R2 = m-tolyl; x = 0; R4 = cyclohexyl] (II) in 28% yield. II inhibited binding of 125I-CCK in rat pancreas and binding of 125I-gastrin in guinea pig gastric glands with IC50's of 1.5 and 0.83 nM, resp. Tablets containing I were prepared

IT 598-41-4P

RN

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of, as intermediate for cholecystokinin and gastrin antagonist)
598-41-4 HCAPLUS

CN Acetamide, 2-amino- (9CI) (CA INDEX NAME)

$$\begin{array}{c} {\rm O} \\ || \\ {\rm H_2N-C-CH_2-NH_2} \end{array}$$

IT 88-19-7 103711-22-4

RL: RCT (Reactant); RACT (Reactant or reagent)

Ι

(reaction of, in preparation of cholecystokinin and gastrin antagonist)

RN 88-19-7 HCAPLUS

CN Benzenesulfonamide, 2-methyl- (9CI) (CA INDEX NAME)

RN 103711-22-4 HCAPLUS

L59 ANSWER 24 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:427154 HCAPLUS

DOCUMENT NUMBER: 117:27154

TITLE: Preparation of antioxidative and antiinflammatory

metal-peptide complexes

INVENTOR(S): Pickart, Loren R.

PATENT ASSIGNEE(S): Procyte Corp., USA

SOURCE: PCT Int. Appl., 44 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

	PATENT NO.					KINI	DATE	APPLICATION NO.		DATE	
	WO	9112				<b>A</b> 1		2 WO 1991-US836		19910207	<
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		RW:	AI,	BE,	CH,	DE,	DK, ES, F	R, GB, GR, IT, LU, NL,	SE		
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	CA	2075	705			AA	199108	.0 CA 1991-2075705		19910207	<
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PRIO	RITY	APP	LN.	INFO	. :			US 1990-478091	Α	19900209	
								WO 1991-US836	Α	19910207	

OTHER SOURCE(S): MARPAT 117:27154

AB Cu(II) and Mn(II) complexes of H-Gly-His-Lys-X [X = aminoalkyl, Trp, (Gly)y-Trp, Pro-X1-Phe-X2, X1-Phe-X2, X3m-Trp, Xn4; m = 4-20; n = 1-5; y = 1-4; X1, X2 = Val, Ala, Gly; X3 = CH2, CH(OH); X4 = glucose, galactose, glucosamine, galactosamine residues], and related compds., were prepared Thus, H-Gly-His-Lys-O(CH2)7Me 1:1 complex with Cu(II), prepared via n-octyl Nɛ-benzyloxycarbonyl-L-lysinate by solution phase coupling, gave 73% inhibition of oxidation of rat liver lipid liposomes mediated by Fe(III)/Fe(II) release from ferritin.

IT 405-39-0 1668-10-6, Glycinamide hydrochloride

# Hoffman 10\_631358

1738-76-7, Benzyl glycinate toluenesulfonate 1738-78-9 16652-76-9, Valine benzyl ester p-toluenesulfonate

35016-67-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(peptide coupling of, in preparation of antioxidant and antiinflammatory peptide-metal complex)

RN 405-39-0 HCAPLUS

CN L-Lysine, N2, N6-bis[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} O & & & \\ \hline Ph & & & \\ O & & & \\ \hline & & & \\ &$$

RN 1668-10-6 HCAPLUS

CN Acetamide, 2-amino-, monohydrochloride (9CI) (CA INDEX NAME)

#### ● HCl

RN 1738-76-7 HCAPLUS

CN Glycine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 1738-68-7 CMF C9 H11 N O2

$$\begin{array}{c} \text{O} \\ || \\ \text{Ph-} \ \text{CH}_2 \text{--} \ \text{O--} \ \text{C--} \ \text{CH}_2 \text{---} \ \text{NH}_2 \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 1738-78-9 HCAPLUS

CN L-Phenylalanine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 962-39-0 CMF C16 H17 N O2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 16652-76-9 HCAPLUS

CN L-Valine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 21760-98-5 CMF C12 H17 N O2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 35016-67-2 HCAPLUS

CN L-Histidine, N,1-bis[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 1138-80-3, Benzyloxycarbonylglycine

RL: RCT (Reactant); RACT (Reactant or reagent)

(peptide coupling of, in preparation of metal-peptide complex antiinflammatory and antioxidant)

RN 1138-80-3 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

$$\begin{array}{c} \text{O} \\ \parallel \\ \text{HO}_2\text{C-CH}_2\text{-NH-C-O-CH}_2\text{-Ph} \end{array}$$

IT 67777-64-4P 136994-56-4P 136994-58-6P

138277-38-0P 138277-42-6P 138277-44-8P

138277-49-3P 138277-50-6P 138277-51-7P

138277-53-9P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for antioxidant and antiinflammatory peptide-metal complex)

RN 67777-64-4 HCAPLUS

CN L-Lysine, N2-[N-[N,1-bis[(phenylmethoxy)carbonyl]-L-histidyl]glycyl]-N6[(phenylmethoxy)carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

## Hoffman 10\_631358

PAGE 1-A

Ph O N H O Ph

O Ph

O Ph

PAGE 1-B

 $\sim_{\mathtt{Ph}}$ 

RN 136994-56-4 HCAPLUS CN Glycine, octyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 94856-68-5 CMF C10 H21 N O2

$$\begin{array}{c} & \text{O} \\ || \\ \text{Me-} & (\text{CH}_2)_7 - \text{O-} \text{C--} \text{CH}_2 - \text{NH}_2 \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 136994-58-6 HCAPLUS

CN Glycine, N-[N-[N2,N6-bis[(phenylmethoxy)carbonyl]-L-lysyl]-1[(phenylmethoxy)carbonyl]-L-histidyl]-, phenylmethyl ester (9CI) (CA
INDEX NAME)

RN 138277-38-0 HCAPLUS

CN Glycinamide, N2,N6-bis[(phenylmethoxy)carbonyl]-L-lysyl-1[(phenylmethoxy)carbonyl]-L-histidyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 138277-42-6 HCAPLUS

CN L-Histidinamide, N-[(phenylmethoxy)carbonyl]glycyl-N-(hexahydro-2-oxo-1H-azepin-4-yl)-1-[(phenylmethoxy)carbonyl]-, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 138277-44-8 HCAPLUS

CN L-Phenylalanine, N-[N2-[N-[N,1-bis[(phenylmethoxy)carbonyl]-L-histidyl]glycyl]-N6-[(phenylmethoxy)carbonyl]-L-lysyl]-, phenylmethylester (9CI) (CA INDEX NAME)

## Hoffman 10\_631358

Absolute stereochemistry.

PAGE 1-B

∕ Ph

RN 138277-49-3 HCAPLUS

CN L-Tryptophan, N-[N2-[N-[N,1-bis[(phenylmethoxy)carbonyl]-L-histidyl]glycyl]-N6-[(phenylmethoxy)carbonyl]-L-lysyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

 $\bigcap_{\mathsf{Ph}}$ 

RN 138277-50-6 HCAPLUS

CN L-Phenylalanine, N-[N2-[N,1-bis[(phenylmethoxy)carbonyl]-L-histidyl]-N6[(phenylmethoxy)carbonyl]-L-lysyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 138277-51-7 HCAPLUS

CN L-Lysine, N2-[N-[N,1-bis[(phenylmethoxy)carbonyl]-L-histidyl]-L-phenylalanyl]-N6-[(phenylmethoxy)carbonyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

\_\_ Ph

RN 138277-53-9 HCAPLUS

CN L-Lysine, N6-[(phenylmethoxy)carbonyl]-N2-[1-[(phenylmethoxy)carbonyl]-N[N-[(phenylmethoxy)carbonyl]-L-alanyl]-L-histidyl]-, phenylmethyl ester
(9CI) (CA INDEX NAME)

L59 ANSWER 25 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1992:59989 HCAPLUS

DOCUMENT NUMBER: 116:59989

TITLE: Preparation of peptide-metal complexes as hair growth

stimulators

INVENTOR(S): Pickart, Loren R.

PATENT ASSIGNEE(S): Procyte Corp., USA

SOURCE: PCT Int. Appl., 42 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 7

PATENT INFORMATION:

									APPLICATION NO.							
WO				<b>A1</b>		1991	0530							19901113	<	
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AU	9168781			A1		1991	10613	A	J 1991	-6878	31			19901113	<	
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EP	500745			A1		1992	0902	E	1990	-9175	577			19901113	<	
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JP	05501567			T2		1993	0325	J	1991	-5005	660			19901113	<	
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								U	3 1992	-9883	352		В1	19921209		

US 1993-101957

B1 19930804

OTHER SOURCE(S):

MARPAT 116:59989

AB Peptide-metal complexes, e.g. H-Gly-His-Lys-R.X (R = NH2, C1-18 alkyl, C6-12 aryl, C1-18 alkoxy, C6-12 aryloxy, Pro-Val-Phe-Val-OH, etc.; X = Cu, Cd, Co, Sn, Fe or Mg ion) and other related peptide-metal complexes, were prepared Thus, H-Lys(Z)-OH was esterified by 1-octanol and the resulting ester was coupled with Boc-His(Z)-OH. The product was deprotected, coupled with Z-Gly-OH, and hydrogenated to give H-Gly-His-Lys-O(CH2)7Me. This was dissolved in H2O and mixed with an equimolar amount of Cu(II) acetate, followed by neutralization by NaOH, to give H-Gly-His-Lys-O(CH2)7Me-copper complex (I). I injected into mice (500 μg/mouse) showed significant acceleration of hair growth for all mice after 2-3 wk.

IT 105132-34-1P 120318-70-9P 136994-47-3P

136994-51-9P 136994-56-4P, Octyl glycinate

p-toluenesulfonate 136994-58-6P

RL: SPN (Synthetic preparation); PREP (Preparation)

(preparation of, as intermediate for preparation of hair growth stimulating peptide-metal complexes)

RN 105132-34-1 HCAPLUS

CN L-Lysine, N6-[(phenylmethoxy)carbonyl]-N2-[1-[(phenylmethoxy)carbonyl]-N[N-[(phenylmethoxy)carbonyl]glycyl]-L-histidyl]-, octyl ester (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 120318-70-9 HCAPLUS

CN L-Lysine, N6-[(phenylmethoxy)carbonyl]-N2-[1-[(phenylmethoxy)carbonyl]-N[N-[(phenylmethoxy)carbonyl]glycyl]-L-histidyl]-, octadecyl ester (9CI)
(CA INDEX NAME)

RN 136994-47-3 HCAPLUS

CN L-Lysinamide, N-[(phenylmethoxy)carbonyl]glycyl-1[(phenylmethoxy)carbonyl]-L-histidyl-N-octyl-N6-[(phenylmethoxy)carbonyl](9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 136994-51-9 HCAPLUS

Absolute stereochemistry.

RN 136994-56-4 HCAPLUS

CN Glycine, octyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 94856-68-5 CMF C10 H21 N O2

$$Me^- (CH_2)_7 - O - C - CH_2 - NH_2$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 136994-58-6 HCAPLUS
CN Glycine, N-[N-[N2,N6-bis[(phenylmethoxy)carbonyl]-L-lysyl]-1 [(phenylmethoxy)carbonyl]-L-histidyl]-, phenylmethyl ester (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.

CN L-Lysine, N2,N6-bis[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$Ph$$

O

N

H

(CH2) 4

S

CO2H

HN

O

Ph

RN 1138-80-3 HCAPLUS CN Glycine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

$$\begin{array}{c} & \text{O} \\ \parallel \\ \text{HO}_2\text{C--} \text{CH}_2 - \text{NH--} \text{C--} \text{O--} \text{CH}_2 - \text{Ph} \end{array}$$

RN 1668-10-6 HCAPLUS

CN Acetamide, 2-amino-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 1738-76-7 HCAPLUS

CN Glycine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 1738-68-7 CMF C9 H11 N O2

$$\begin{array}{c} & \text{O} \\ || \\ \text{Ph-CH}_2\text{--O-C-CH}_2\text{--NH}_2 \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 2212-75-1 HCAPLUS

CN L-Lysine, N2-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 16652-76-9 HCAPLUS

CN L-Valine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME) CM 1

CRN 21760-98-5 CMF C12 H17 N O2

Absolute stereochemistry. Rotation (-).

CM2

CRN 104-15-4 CMF C7 H8 O3 S

L59 ANSWER 26 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1991:164815 HCAPLUS

DOCUMENT NUMBER:

114:164815

TITLE:

Preparation of peptides as antidementia agents

INVENTOR(S):

Masaki, Mitsuo; Uehara, Masaki; Hirate, Kenji; Isowa,

Yoshikazu; Sato, Yoshiaki; Nakashima, Yoshiharu

PATENT ASSIGNEE(S):

Nippon Chemiphar Co., Ltd., Japan; Fujirebio, Inc.

SOURCE:

Eur. Pat. Appl., 36 pp.

CODEN: EPXXDW

DOCUMENT TYPE:

Patent

LANGUAGE:

English

FAMILY ACC. NUM. COUNT:

2

PATENT INFORMATION:

PATENT NO.			KIN	D DA	TE		API	PLICAT	DATE					
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#### Hoffman 10 631358

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    AU 9053621
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PRIORITY APPLN. INFO.:
                                            JP 1989-95917
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                                            JP 1989-95921
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                                            JP 1989-95922
                                                               A3 19900412
                                            EP 1990-303987
                                            US 1990-509950
                                                               A3 19900416
```

OTHER SOURCE(S): MARPAT 114:164815

Ι

H-pGlu-Asn-Cys-A-B-Gly-OH | | H-Cys-OH

AB The title peptides [I; A = D- or L-Pro and B = citrulline (Cit) or homoarginine (Har) residue; A = D-Pro, B = Arg; A = Sar, pipecolic acid residue (Pip), azetidine-2-carboxylic acid (Aze), or Arg, B = D- or L-Arg], H-Asn-A-L- (or D-) Pro-Arg-(Gly)nOH (A = Ser, Thr, Ala; n = 0, 1), A-Ser-Pip-Arg-OH (A = H-Pro-Asn, H-Asn, H-Pro), A-Cys(W)-Pro-Arg-B [A = cyclopentylcarbonyl, H-Pro, H-pGlu (pGlu = pyroglutamic acid residue); B = Gly-OH,  $\beta$ -Ala-OH; W = H, S-linked H-Cys-OH or (A-Cys-Pro-Arg-B)2], H-pGlu-Asn-Ser-A-B-(Gly)nOH (A = Aze, D- or L-Pro, Pip, Ser; B = D- or L-Arg, Cit, Har, Lys, Orn; n = 0, 1), H-Pro-(Asn)m-Ser-L-(or D-)-Pro-Arg-(Gly)nOH (m, n = 0, 1), and H-Pro-(Asn)m-Ser-L-(or D-)-Pro-Arg-(Gly)nOH (n = 0, 1), having a nootropic effect superior to vasopressin, were prepared Approx. 30 peptides were prepared by the solution method and 8 peptides at 0.1 and 1 ng/kg showed 213-460% improvement effect on memory consolidation in retrograde amnesia induced by a electro-shock and cycloheximide. Injection, collunarium, and suppository formulations containing the title peptides are given.

IT 1668-10-6, Glycinamide hydrochloride 2304-96-3 27019-47-2,  $\beta$ -Alanine benzyl ester p-toluenesulfonate 58810-11-0

RL: RCT (Reactant); RACT (Reactant or reagent)

(peptide coupling of, in preparation of antidementia peptide)

RN 1668-10-6 HCAPLUS

CN Acetamide, 2-amino-, monohydrochloride (9CI) (CA INDEX NAME)

● HCl

RN 2304-96-3 HCAPLUS

CN L-Asparagine, N2-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 27019-47-2 HCAPLUS

CN  $\beta$ -Alanine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 14529-00-1 CMF C10 H13 N O2

$$\begin{array}{c|c} & \text{O} & \\ \parallel & \\ \text{Ph-} & \text{CH}_2\text{--} & \text{O-} & \text{C--} & \text{CH}_2\text{--} & \text{CH}_2\text{--} & \text{NH}_2 \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 58810-11-0 HCAPLUS

CN L-Ornithine, N5-[imino[[(4-methoxyphenyl)sulfonyl]amino]methyl]-N2[(phenylmethoxy)carbonyl]-, compd. with N-cyclohexylcyclohexanamine (1:1)
(9CI) (CA INDEX NAME)

CM 1

CRN 58810-10-9 CMF C21 H26 N4 O7 S

### Absolute stereochemistry.

CM 2

CRN 101-83-7 CMF C12 H23 N

IT 88333-77-1P 132925-86-1P 132925-88-3P

132925-90-7P 132925-92-9P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for antidementia peptide)

RN 88333-77-1 HCAPLUS

CN Glycinamide, N5-[imino[[(4-methoxyphenyl)sulfonyl]amino]methyl]-N2-[(phenylmethoxy)carbonyl]-L-ornithyl- (9CI) (CA INDEX NAME)

### Absolute stereochemistry.

RN 132925-86-1 HCAPLUS

CN L-Ornithine, N5-[imino(nitroamino)methyl]-N2-[1-[N-[N2-[(phenylmethoxy)carbonyl]-L-asparaginyl]-O-(phenylmethyl)-L-seryl]-Lprolyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 132925-88-3 HCAPLUS

CN L-Ornithine, N5-[imino(nitroamino)methyl]-N2-[1-[N-[N2-[(phenylmethoxy)carbonyl]-L-asparaginyl]-L-threonyl]-L-prolyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 132925-90-7 HCAPLUS

CN L-Ornithine, N5-[imino(nitroamino)methyl]-N2-[1-[N-[N2-[(phenylmethoxy)carbonyl]-L-asparaginyl]-L-alanyl]-L-prolyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 132925-92-9 HCAPLUS

CN L-Ornithine, N5-[imino(nitroamino)methyl]-N2-[1-[N-[N2-[(phenylmethoxy)carbonyl]-L-asparaginyl]-O-(phenylmethyl)-L-seryl]-Dprolyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L59 ANSWER 27 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:179892 HCAPLUS

DOCUMENT NUMBER: 112:179892

TITLE: Polypeptides stabilized by covalent hydrogen bond

replacements

INVENTOR(S): Satterthwait, Arnold C., Jr.; Arrhenius, Thomas

PATENT ASSIGNEE(S): Scripps Clinic and Research Foundation, USA

SOURCE: Eur. Pat. Appl., 27 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 336779	A2	19891011	EP 1989-303469	19890407 <
EP 336779	A3	19910821		
R: AT, BE, CH,	DE, ES	, FR, GB, G	GR, IT, LI, LU, NL, SE	
WO 8909783	A1	19891019	WO 1989-US1452	19890407 <

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W: AU, DK, JP
    AU 8935349
                          A1
                                19891103
                                            AU 1989-35349
                                                                   19890407 <--
                                                                   19890407 <--
     JP 03504496
                          T2
                                19911003
                                            JP 1989-504770
    DK 9002411
                          Α
                                19901207
                                            DK 1990-2411
                                                                   19901005 <--
    US 5807979
                          Α
                                19980915
                                            US 1995-456424
                                                                   19950601 <--
PRIORITY APPLN. INFO.:
                                            US 1988-179160
                                                              A 19880408
                                            WO 1989-US1452
                                                               A 19890407
                                            US 1990-607645
                                                               B1 19901029
                                            US 1991-746064
                                                               B2 19910812
                                            US 1992-866040
                                                                B1 19920408
                                            US 1994-224059
                                                                B1 19940407
OTHER SOURCE(S):
                        MARPAT 112:179892
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GI

AB Peptides [I; X = H, halo, C1-6 (halo)alkyl, C1-6 acyl, PhCH2, amino acid sequence of 1-40 amino acids; m = 1-6; X1 = amino acid sequence of 1-12 amino acids], (II; R = C1-6 alkoxy, PhO, naphthyloxy, BzO, NH2; X2 = amino acid sequence of 1-12 amino acids; m = 1-6) and (III; X3, X4 = amino acid sequences of 1-12 amino acids), which are stabilized and restricted to particular conformations in solution by replacing one or more hydrogen bonds with covalent hydrogen bond mimics, i.e. IV and V, and thus show enhanced biol. activities, e.g. as hormones and vaccines, are prepared by determination of an

approx. three-dimensional structure for the active region of a peptide, identification of a stabilizing hydrogen bond, and preparation of a peptide having the same amino sequence as the active region of the peptide and also containing the covalent hydrogen bond mimics, IV or V. The synthesis of the IV and V mimics involves reactions of a peptide containing thioamide NHC(S) with MeI to form +NH:C(SMe) followed by reaction with a peptide containing NCH2NH2 to give IV or reaction of a CH2CHCH(OMe)2 peptide analog side chain with a peptide containing NNH2 to give V. Thus, cyclization of MeC(SMe):N+Me-Glu-Ser-Leu-NHCH2CH2N+H3 in DMF by treatment with a weakly basic ion exchanger gave a reverse-turn stabilized epidermal growth factor analog I (X = Me, X1 = Ala-Ala, m = 1) of high activity.

ΙT 1738-77-8 RL: RCT (Reactant); RACT (Reactant or reagent)
 (acylation of, by dimethoxypentanoic acid)

RN 1738-77-8 HCAPLUS

CN L-Leucine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 1738-69-8 CMF C13 H19 N O2

Absolute stereochemistry.

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

IT 1142-20-7

RL: RCT (Reactant); RACT (Reactant or reagent)

(esterification of, with hydroxysuccinimide, in preparation of stabilized peptide)

RN 1142-20-7 HCAPLUS

CN L-Alanine, N-[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 3235-17-4P 3401-36-3P 126166-00-5P

126166-01-6P 126166-08-3P 126166-10-7P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as intermediate for peptide stabilized by covalent hydrogen

RN 3235-17-4 HCAPLUS

bond mimic)

CN Glycine, N-[(phenylmethoxy)carbonyl]-L-alanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 3401-36-3 HCAPLUS

CN Carbamic acid, [(1S)-2-[(2,5-dioxo-1-pyrrolidinyl)oxy]-1-methyl-2-oxoethyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 126166-00-5 HCAPLUS

CN 9-Oxa-2,5,7-triazaundecanoic acid, 3,10,10-trimethyl-4,8-dioxo-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 126166-01-6 HCAPLUS

CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-N-[[[(1,1-dimethylethoxy)carbonyl]amino]methyl]- (9CI) (CA INDEX NAME)

## Hoffman 10\_631358

Synthetic studies on copper(II)-transporting peptides. TITLE:

I. An improved synthesis of Gly-His-Lys and some its

analogs

AUTHOR(S):

Iwai, Michio

CORPORATE SOURCE:

Mar. Tech. Coll., Ashiya, Japan

SOURCE:

Kaigi Daigakko Kenkyu Hokoku (1988), 31,

33-43

CODEN: KDAKAR; ISSN: 0288-3708

DOCUMENT TYPE:

Journal

LANGUAGE:

Japanese

Cu(II)-transporting peptide H-Gly-His-Lys-OH and analogs H-Gly-His-Orn-OH, AB H-His-Lys-Gly-OH, and H-Pro-Leu-Gly-NH2 were prepared by stepwise couplings in solution

TT 35016-67-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(peptide coupling of, with dipeptide derivative)

RN 35016-67-2 HCAPLUS

L-Histidine, N,1-bis[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME) CN

Absolute stereochemistry.

IT 1138-80-3

> RL: RCT (Reactant); RACT (Reactant or reagent) (peptide coupling of, with dipeptide derivs.)

RN 1138-80-3 HCAPLUS

Glycine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME) CN

IT 598-41-4, Glycinamide

> RL: RCT (Reactant); RACT (Reactant or reagent) (peptide coupling of, with leucine derivative)

RN598-41-4 HCAPLUS

Acetamide, 2-amino- (9CI) (CA INDEX NAME) CN

IT 1738-76-7, Glycine benzyl ester tosylate

> RL: RCT (Reactant); RACT (Reactant or reagent) (peptide coupling of, with lysine derivative)

RN1738-76-7 HCAPLUS

CN Glycine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

RN 126166-08-3 HCAPLUS

CN 10-Oxa-2,5,8-triazadodecanoic acid, 3,11,11-trimethyl-4,9-dioxo-, phenylmethyl ester, (3S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 126166-10-7 HCAPLUS

CN L-Alaninamide, N-[(phenylmethoxy)carbonyl]-L-alanyl-N-[2-[[(1,1-dimethylethoxy)carbonyl]amino]ethyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 107-15-3, 1,2-Ethanediamine, reactions

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, in preparation of conformationally restricted peptide analogs)

RN 107-15-3 HCAPLUS

CN 1,2-Ethanediamine (9CI) (CA INDEX NAME)

H2N-CH2-CH2-NH2

L59 ANSWER 28 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1989:39348 HCAPLUS

DOCUMENT NUMBER: 110:39348

CM 1

CRN 1738-68-7 CMF C9 H11 N O2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

IT 118349-24-9P 118349-28-3P 118349-30-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenolysis of)

RN 118349-24-9 HCAPLUS

CN L-Lysine, N6-[(phenylmethoxy)carbonyl]-N2-[N-[N-[(phenylmethoxy)carbonyl]glycyl]-1-(phenylmethyl)-L-histidyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 118349-28-3 HCAPLUS

CN L-Ornithine, N5-[(phenylmethoxy)carbonyl]-N2-[N-[N-[(phenylmethoxy)carbonyl]glycyl]-1-(phenylmethyl)-L-histidyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

RN 118349-30-7 HCAPLUS

CN Glycine, N-[N2-[N,1-bis[(phenylmethoxy)carbonyl]-L-histidyl]-N6[(phenylmethoxy)carbonyl]-L-lysyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

L59 ANSWER 29 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1987:102683 HCAPLUS

DOCUMENT NUMBER: 106:102683

TITLE:  $\alpha$ -Human Atrial Natriuretic polypeptide ( $\alpha$ -

hANP) analogs

INVENTOR(S): Kiso, Yoshiaki; Shimokura, Masanori; Hosoi, Satoru;

Fujisaki, Toshio

PATENT ASSIGNEE(S): Abbott Laboratories, USA SOURCE: Jpn. Kokai Tokkyo Koho, 14 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

APPLICATION NO. PATENT NO. KIND DATE DATE \_\_\_\_\_\_ \_\_\_\_\_ -----\_ \_ \_ \_ <del>-</del>----JP 61243100 A2 19861029 JP 1985-82692 19850419 <--JP 1985-82692 19850419 PRIORITY APPLN. INFO.: GI

The title compds. [I; X = D-Met, L-Leu, Ile, Nle; Xl = NHCH(CONH2)CH2S2CH2CH(NH2)CO, NH(CH2)nCO(n = 1-10)], useful as antihypertensives, diuretics and natriuretics, were prepared by the solution method. I at 10  $\mu$ g in vivo i.v. increased urine, Na and K excretion through kidneys by 37  $\pm$  8, 99  $\pm$  58, and 54  $\pm$  14%, resp., without changing the blood pressure and with a slight increase (13  $\pm$  6%) in blood flow through kidneys in rats.

IT 1738-76-7, Glycine benzyl ester p-toluenesulfonic acid salt 4427-49-0 23234-83-5,
N-(p-Methoxybenzyloxycarbonyl)leucine 23336-96-1 23931-71-7 53049-30-2 89821-13-6 99236-54-1 99236-56-3 99236-59-6

106487-75-6 106487-79-0 106983-89-5 106983-91-9 106983-94-2

106983-91-9 106983-94-2 PL. PCT (Peactant) · PAC

RL: RCT (Reactant); RACT (Reactant or reagent) (peptide coupling of, in preparation of  $\alpha$ -human atrial natriuretic polypeptide analog)

RN 1738-76-7 HCAPLUS

CN Glycine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 1738-68-7 CMF C9 H11 N O2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 4427-49-0 HCAPLUS

CN L-Aspartic acid, N-[[(4-methoxyphenyl)methoxy]carbonyl]-, 4-(phenylmethyl)
 ester (9CI) (CA INDEX NAME)

$$\begin{array}{c|c} & & & & \\ & & & \\ \hline \\ MeO \end{array}$$

RN 23234-83-5 HCAPLUS

CN L-Leucine, N-[[(4-methoxyphenyl)methoxy]carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 23336-96-1 HCAPLUS

CN L-Alanine, N-[[(4-methoxyphenyl)methoxy]carbonyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 23931-71-7 HCAPLUS

CN L-Glutamine, N2-[[(4-methoxyphenyl)methoxy]carbonyl]-, 4-nitrophenyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2N$$
 $O$ 
 $S$ 
 $N$ 
 $O$ 
 $OMe$ 

RN 53049-30-2 HCAPLUS

CN L-Aspartic acid, N-[[(4-methoxyphenyl)methoxy]carbonyl]-,

1-(4-nitrophenyl) 4-(phenylmethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 89821-13-6 HCAPLUS

CN L-Leucine, N-[N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-N2[[(4-methoxyphenyl)methoxy]carbonyl]-L-ornithyl]-, hydrazide (9CI) (CA
INDEX NAME)

Absolute stereochemistry.

RN 99236-54-1 HCAPLUS

CN Glycine, N-[N-[N2-[N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-alanyl]-L-glutaminyl]-L-seryl]-, hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 99236-56-3 HCAPLUS

CN Butanoic acid, N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-N2-[((4-methoxyphenyl)methoxy]carbonyl]-L-ornithyl-4-(methylsulfinyl)-L-2amino-, hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 99236-59-6 HCAPLUS

CN Glycine, N-[N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-leucyl]-, hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 106487-75-6 HCAPLUS

CN Glycine, N-[N-[N-[N-[(4-methoxyphenyl)methoxy]carbonyl]-S-[(2,4,6trimethylphenyl)methyl]-L-cysteinyl]-L-phenylalanyl]glycyl]-, hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 106487-79-0 HCAPLUS

CN Glycine, N-[N-[N-[(4-methoxyphenyl)methoxy]carbonyl]-Lphenylalanyl]glycyl]-, hydrazide (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 106983-89-5 HCAPLUS

CN Carbamic acid, [2-amino-2-oxo-1-[[[(2,4,6-trimethylphenyl)methyl]thio]methyl]ethyl]-, (4-methoxyphenyl)methyl ester, (R)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 106983-91-9 HCAPLUS

CN Glycine, N-[N-[N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-N2[[(4-methoxyphenyl)methoxy]carbonyl]-L-ornithyl]-L-isoleucyl]-, hydrazide
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 106983-94-2 HCAPLUS

CN L-Methionine, N-[N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]N2-[[(4-methoxyphenyl)methoxy]carbonyl]-L-ornithyl]-, hydrazide (9CI) (CA
INDEX NAME)

IT 106983-85-1P

CN

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and deprotection and cyclization of,  $\alpha$ -human atrial natriuretic polypeptide analog from)

RN 106983-85-1 HCAPLUS

3-19-Atrial natriuretic peptide-21 (rat reduced), 3-[N-[[(4-methoxyphenyl)methoxy]carbonyl]-S-[(2,4,6-trimethylphenyl)methyl]-L-cysteine]-7-[N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithine]-8-L-leucine-10-[N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithine]-19-[S-[(2,4,6-trimethylphenyl)methyl]-L-cysteinamide]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B Me Me. Н HN; 0 (CH<sub>2</sub>) 3 NH Me i-Bu Н N H Н Н 0 Ô 0 Me Me Εt Ph

PAGE 1-C

PAGE 2-A

Me

Me

Me

IT 82882-73-3P 106487-77-8P 106487-80-3P 106983-88-4P 106983-90-8P 106983-91-9P 106983-92-0P 106983-93-1P 106983-95-3P 106983-96-4P 106983-98-6P 106983-99-7P 106984-00-3P 106984-01-4P 107052-98-2P RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent) (preparation and peptide coupling of, in preparation of  $\alpha$ -human atrial natriuretic polypeptide analog) 82882-73-3 HCAPLUS

RN 82882-73-3 HCAPLUS
CN Glycine, N-[N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-leucyl]-,
 phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 106487-77-8 HCAPLUS

CN L-Cysteinamide, N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-alanyl-L-glutaminyl-L-serylglycyl-L-leucylglycyl-S-[(2,4,6-trimethylphenyl)methyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-B

RN 106487-80-3 HCAPLUS

CN Glycine, N-[N-[N-[N-[N-[N-[((4-methoxyphenyl)methoxy]carbonyl]-L-alanyl] L-glutaminyl]-O-(phenylmethyl)-L-seryl]glycyl]-L-leucyl]- (9CI) (CA INDEX NAME)

Hoffman 10\_631358

0

Me H S Ph O Ph O Ph O Ph

PAGE 1-B

PAGE 1-A

-  $\stackrel{\text{H}}{\text{N}}$   $CO_2H$ 

∕Bu-i

MeO

RN 106983-88-4 HCAPLUS

CN L-Cysteinamide, N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-leucylglycyl-S[(2,4,6-trimethylphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A
e Me H<sub>2</sub>N O

PAGE 1-B

<sup>\_</sup>OMe

RN 106983-90-8 HCAPLUS

CN L-Cysteinamide, N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-N2-[[(4-methoxyphenyl)methoxy]carbonyl]-L-ornithyl-L-isoleucylglycyl-L-alanyl-L-glutaminyl-L-serylglycyl-L-leucylglycyl-S-[(2,4,6-trimethylphenyl)methyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

Me 
$$H_2N$$
 $M_1$ 
 $M_2N$ 
 $M_1$ 
 $M_2$ 
 $M_1$ 
 $M_2$ 
 $M_3$ 
 $M_4$ 
 $M_4$ 
 $M_5$ 
 $M_4$ 
 $M_5$ 
 $M_6$ 
 $M_6$ 

PAGE 1-B

PAGE 1-C

<sup>\_</sup>OMe

RN 106983-91-9 HCAPLUS

CN Glycine, N-[N-[N5-[imino[((2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-N2[[(4-methoxyphenyl)methoxy]carbonyl]-L-ornithyl]-L-isoleucyl]-, hydrazide
(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 106983-92-0 HCAPLUS

CN L-Cysteinamide, N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-α-aspartylN5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithyl-Lisoleucylglycyl-L-alanyl-L-glutaminyl-L-serylglycyl-L-leucylglycyl-S[(2,4,6-trimethylphenyl)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

# PAGE 1-A

# PAGE 1-B

# PAGE 1-C

RN 106983-93-1 HCAPLUS

CN L-Cysteinamide, N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-methionyl-L-  $\alpha$ -aspartyl-N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithyl-L-isoleucylglycyl-L-alanyl-L-glutaminyl-L-serylglycyl-L-leucylglycyl-S-[(2,4,6-trimethylphenyl)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

PAGE 1-C

RN 106983-95-3 HCAPLUS

CN 3-19-Atrial natriuretic peptide-21 (human reduced), 3-[N-[[(4-methoxyphenyl)methoxy]carbonyl]-S-[(2,4,6-trimethylphenyl)methyl]-L-cysteine]-7-[N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithine]-10-[N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithine]-19-[S-[(2,4,6-trimethylphenyl)methyl]-L-cysteinamide]- (9CI) (CA INDEX NAME)

# PAGE 1-B

# PAGE 1-C

PAGE 1-D

RN 106983-96-4 HCAPLUS

CN L-Cysteinamide, N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-N2-[[(4-methoxyphenyl)methoxy]carbonyl]-L-ornithyl-L-leucyl-L-α-aspartyl-N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithyl-L-isoleucylglycyl-L-alanyl-L-glutaminyl-L-serylglycyl-L-leucylglycyl-S-[(2,4,6-trimethylphenyl)methyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 1-C

$$\begin{array}{c|c} & & & & \\ & & & \\ N & & & \\ N & & \\ N & & \\ \end{array}$$

RN 106983-98-6 HCAPLUS

CN Glycine, N-[N-[N-[N-[N2-[[(4-methoxyphenyl)methoxy]carbonyl]-L-glutaminyl]-O-(phenylmethyl)-L-seryl]glycyl]-L-leucyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c}
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RN 106983-99-7 HCAPLUS

Hoffman 10 631358

Absolute stereochemistry.

PAGE 1-B

#### PAGE 1-A

#### PAGE 1-B

RN 106984-01-4 HCAPLUS

CN Glycine, N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-N2-[[(4-methoxyphenyl)methoxy]carbonyl]-L-ornithyl-4-(methylsulfinyl)-L-2aminobutanoyl-L-α-aspartyl-N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithyl-L-isoleucylglycyl-Lalanyl-L-glutaminyl-O-(phenylmethyl)-L-serylglycyl-L-leucyl-,
3-(phenylmethyl) ester (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

RN 107052-98-2 HCAPLUS

CN Glycine, N-[[(4-methoxyphenyl)methoxy]carbonyl]-L-phenylalanylglycylglycyl-N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithyl-4-(methylsulfinyl)-L-2-aminobutanoyl-L-α-aspartyl-N5-[imino[[(2,4,6-trimethylphenyl)sulfonyl]amino]methyl]-L-ornithyl-L-isoleucylglycyl-L-alanyl-L-glutaminyl-O-(phenylmethyl)-L-serylglycyl-L-leucyl-, 6-(phenylmethyl) ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 1-C

L59 ANSWER 30 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1986:553560 HCAPLUS

DOCUMENT NUMBER: 105:153560

TITLE: Modified tripeptides

INVENTOR(S):
Nicolaides, Ernest D.; Tinney, Francis J.;

Kaltenbronn, James S.; DeJohn, Dana E.; Lunney, Elizabeth A.; Roark, W. Howard; Repine, Joseph T.

PATENT ASSIGNEE(S): Warner-Lambert Co., USA

SOURCE: U.S., 28 pp.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4596819	Α	19860624	US 1984-573233	19840123 <
PRIORITY APPLN. INFO.:			US 1984-573233	19840123
GT				

Proline peptide analogs I (R1 = H, CO2CH2Ph, CO2CMe3, etc.; R2 = H, CH2CHMe2; R3 = CO2H, carbalkoxy, CONH2, CO2CH2Ph, CONHCH2CO2H, etc.) were prepared, and they exhibited amnesia reversal properties in rats and mice. Prolinol was N-acylated by Me2CHCH2CHBrCOCl, the product was cyclized, and the pyrrolo[2,1-c][1,4]oxazine derivative obtained was converted, in a series of reactions, to peptide analog II.

## Hoffman 10\_631358

IT 55456-48-9P 67488-65-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of)

RN 55456-48-9 HCAPLUS

CN 2-Pyrrolidinemethanol, 1-[(4-methylphenyl)sulfonyl]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 67488-65-7 HCAPLUS

CN L-Proline, 1-[(4-methylphenyl)sulfonyl]-, methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 98-59-9 1668-10-6 2018-66-8 6401-56-5

51077-01-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of)

RN 98-59-9 HCAPLUS

CN Benzenesulfonyl chloride, 4-methyl- (9CI) (CA INDEX NAME)

RN 1668-10-6 HCAPLUS

CN Acetamide, 2-amino-, monohydrochloride (9CI) (CA INDEX NAME)

HCl

RN 2018-66-8 HCAPLUS

CN L-Leucine, N-[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 6401-56-5 HCAPLUS

Absolute stereochemistry.

RN 51077-01-1 HCAPLUS

CN L-Proline, 1-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

L59 ANSWER 31 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

#### Hoffman 10 631358

1986:186822 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 104:186822

Synthesis and biological activity of linear and cyclic TITLE:

> enkephalins modified at the Gly3-Phe4 amide bond Richman, S. J.; Goodman, M.; Nguyen, Thi M. D.;

Schiller, P. W.

CORPORATE SOURCE: Dep. Chem., Univ. California, San Diego, La Jolla, CA,

USA

SOURCE: International Journal of Peptide & Protein Research (

1985), 25(6), 648-62 CODEN: IJPPC3; ISSN: 0367-8377

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 104:186822 For diagram(s), see printed CA Issue.

AB As part of a continuing effort to define structure-activity relationships for enkephalin and design enzymically resistant analogs, the partial retro-inverso enkephalin analog H-Tyr-D-Ala-gGly-(R,S)-mPhe-Leu-NH2 [mPhe = OCCH(CH2Ph)CO, gGly = NHCH2NH] and its cyclic counterpart I were synthesized as diastereomeric mixts. using solution methodol. The racemic benzylmalonate allowed the linear analog to be synthesized by fragment coupling at the reversed bond. Cyclization of the second analog was carried out at high concentration, eliminating formation of polymer by the use

of an insol. base. All gem-diaminoalkyl residues were prepared by conversion of peptide amides with benzene iodonium bis(trifluoroacetate). Diastereomers of both compds. were separable by reverse phase HPLC, but those of the linear compound racemized rapidly under conditions of testing

and were therefore tested together. All analogs tested had activities ranging from 6 to 14% of the activity of Leu-enkephalin, indicating that the Gly3-Phe4 amide bond is important, though not crucial, for receptor binding.

1738-77-8

AUTHOR (S):

IT RL: RCT (Reactant); RACT (Reactant or reagent)

(coupling of, with benzyl malonic acid derivative)

1738-77-8 HCAPLUS RN

L-Leucine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX CN NAME)

CM 1

CRN 1738-69-8 CMF C13 H19 N O2

Absolute stereochemistry.

CM

CRN 104-15-4 CMF C7 H8 O3 S

IT 1668-10-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(peptide coupling of)

RN 1668-10-6 HCAPLUS

CN Acetamide, 2-amino-, monohydrochloride (9CI) (CA INDEX NAME)

### ● HCl

IT 26607-51-2

RL: RCT (Reactant); RACT (Reactant or reagent)

(peptide coupling of, with glycinamide)

RN 26607-51-2 HCAPLUS

CN D-Alanine, N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

$$HN$$
  $O$   $Ph$   $HO_2C$   $R$   $Me$ 

IT 101854-67-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and hydrogenolysis of)

RN 101854-67-5 HCAPLUS

CN Glycinamide, N-[(phenylmethoxy)carbonyl]-D-alanyl- (9CI) (CA INDEX NAME)

L59 ANSWER 32 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER:

1983:402694 HCAPLUS

DOCUMENT NUMBER:

99:2694

TITLE:

Critical examination of a method for the analysis of

 $\alpha$  and  $\omega$  linkages in peptides containing

aspartic acid and glutamic acid

AUTHOR(S): CORPORATE SOURCE: Capecchi, John T.; Miller, Marvin J.; Loudon, G. Marc Sch. Pharm. Pharm. Sci., Purdue Univ., West Lafayette,

IN, 47907, USA

SOURCE:

Journal of Organic Chemistry (1983), 48(12),

2014-21

CODEN: JOCEAH; ISSN: 0022-3263

DOCUMENT TYPE:

Journal English

LANGUAGE:

Coupling of O-pivaloylhydroxylamine and subsequent Lossen rearrangement under mild conditions led to the disappearance of  $\beta$ -aspartyl and  $\gamma$ -glutamyl residues from subsequent amino acid anal. in a variety of peptides. Residues from the usual  $\alpha$  linkage rearrange much more sluggishly to products that are detectable by amino acid anal. An interesting complication in the procedure is that  $\alpha$ -linked glutamyl residues are converted in part to a 2-oxohexahydropyrimidine-4-carboxylic acid derivative which is stable to extended acid hydrolysis. After base hydrolysis, this derivative yields 2,4-diaminobutanoic acid. This reaction explains aberrant results in the linkage anal. of collagen that has been reported in the literature.

IT 85701-66-2P 85701-67-3P 85701-68-4P 85701-69-5P 85701-70-8P 85701-71-9P

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenolysis of)

RN 85701-66-2 HCAPLUS

CN L-Valine, N-[N-[(phenylmethoxy)carbonyl]-L- $\alpha$ -glutamyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 85701-67-3 HCAPLUS

CN L-Valine, N-[N-[(phenylmethoxy)carbonyl]-L-γ-glutamyl]- (9CI) (CA
INDEX NAME)

RN 85701-68-4 HCAPLUS

CN L-Leucine, N-[N-[N-[(phenylmethoxy)carbonyl]-L- $\alpha$ -glutamyl]-L-alanyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 85701-69-5 HCAPLUS

CN L-Leucine, N-[N-[N-[(phenylmethoxy)carbonyl]-L- $\gamma$ -glutamyl]-L-alanyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 85701-70-8 HCAPLUS

CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]-L- $\alpha$ -glutamyl- (9CI) (CA INDEX NAME)

RN 85701-71-9 HCAPLUS

CN L-Leucinamide, N-[(phenylmethoxy)carbonyl]-L-γ-glutamyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 2886-33-1

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with acetylphenylalanine hydroxysuccinimide ester)

RN 2886-33-1 HCAPLUS

CN L-Aspartic acid, bis(phenylmethyl) ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 2791-79-9 CMF C18 H19 N O4

Absolute stereochemistry. Rotation (+).

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

IT 1668-10-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with benzyl acetylphenylalanylaspartate)

RN 1668-10-6 HCAPLUS

CN Acetamide, 2-amino-, monohydrochloride (9CI) (CA INDEX NAME)

$$^{\rm O}_{\rm ||}_{\rm H_2N-C-CH_2-NH_2}$$

#### HCl

L59 ANSWER 33 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1982:223296 HCAPLUS

DOCUMENT NUMBER: 96:223296

TITLE: Use of peptides as anti-sickling agents

INVENTOR(S): Collinson-Jones, Rosalind Isabel; Pardon, John

Frederick

PATENT ASSIGNEE(S): G.D. Searle and Co., UK

SOURCE: Brit. UK Pat. Appl., 14 pp.

CODEN: BAXXDU

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

7 2000014 3 1000010	
GB 2080684 A 19820210 GB 1981-23542 19810731 < US 4376766 A 19830315 US 1981-286416 19810724 <	
PRIORITY APPLN. INFO.: GB 1980-25178 A 19800801	
AB An antisickling composition consists of 1 or more of L-lysine-L-phenylalanin (I) [6235-35-4], L-lysine-L-tyrosine [35978-98-4], L-histidine-L-lysine-L-tyrosine-L-histidine [81839-28-3] and their salts in addition to pharmaceutically-acceptable carriers, diluents and adjuvants. These peptides inhibit the gelation of deoxygenated sickle cell Hb solution in vitro. The solubility of deoxygenated sickle cell Hb is increased in the presence of the antisickling agent to a level comparable to that of Hb from heterologous trait blood. The number of cells sickling at low 0 pressures is decreased by incubation with I. Thus, a mixture of L-phenylalanine [63-91-2], p-toluenesulfonic acid, benzyl alc. on refluxing gave L-phenylalanine benzyl ester p-toluenesulfonate [1738-78-9] which was condensed with a,s-dicarbobenzoxy-L-lysine [405-39-0] in the presence of iso-Bu chloroformate and Et3N. This protected peptide was subjected to hydrogenolysis and hydrolysis in the presence 10% Pd-C in formic acid and MeOH. Acidification yielded I.2HCl [81839-29-4]. The peptides may be used in conventional slow-release formulations.	ne

IT 1667-92-1P

RL: RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(preparation and hydrogenolysis and hydrolysis of)

RN 1667-92-1 HCAPLUS

CN L-Phenylalanine, N-[N2,N6-bis[(phenylmethoxy)carbonyl]-L-lysyl]-,
 phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 405-39-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with benzyl phenylalanine p-toluenesulfonate)

RN 405-39-0 HCAPLUS

CN L-Lysine, N2, N6-bis[(phenylmethoxy)carbonyl] - (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$Ph$$

O

N

H

(CH2) 4

S

CO2H

HN

O

Ph

IT 1738-78-9P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, with dicarbobenzoxylysine)

RN 1738-78-9 HCAPLUS

CN L-Phenylalanine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 962-39-0

CMF C16 H17 N O2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L59 ANSWER 34 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1980:550378 HCAPLUS

DOCUMENT NUMBER: 93:150378

TITLE: Hydroxyaminoalkylphosphonic acids

INVENTOR(S): Hashimoto, Masashi; Hemmi, Keiji; Kamiya, Takashi;

Takeno, Hidekazu

PATENT ASSIGNEE(S): Fujisawa Pharmaceutical Co., Ltd., Japan

SOURCE: U.S., 38 pp. Cont.-in-part of U.S. Ser. No. 819,554.

CODEN: USXXAM

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4206156	 А	19800603	US 1978-897303	19780417 <
GB 1580899	Α	19801210	GB 1976-31339	19760727 <
ZA 7704528	Α	19790228	ZA 1977-4528	19770726 <
CA 1103179	A1	19810616	CA 1977-283479	19770726 <- <i>-</i>
BE 857211	A1	19771114	BE 1977-179680	19770727 <
US 4143135	Α	19790306	US 1977-819551	19770727 <
US 4182758	A	19800108	US 1977-819554	19770727 <
CH 647807	Α	19850215	CH 1984-427	19770727 <
CH 643857	Α	19840629	CH 1978-12607	19781211 <
ES 479210	A1	19791216	ES 1979-479210	19790402 <
ES 479212	A1	19791216	ES 1979-479212	19790402 <
AT 7905646	Α	19811115	AT 1979-5646	19790822 <
AT 367428	В	19820712		
AT 7905647	Α	19811115	AT 1979-5647	19790822 <
AT 367429	В	19820712		
AT 7905648	Α	19811115	AT 1979-5648	19790822 <
AT 367430	В	19820712		
DK 8102666	Α	19810617	DK 1981-2666	19810617 <
DK 149822	В	19861006		
DK 149822	С	19870323		

A
B
19c
C
19851
A
1982051c
B
19860606
C
19860924
A
19830120
SF
B
19880201
C
19880519
A
19841228
A
19841228
A
19841228 Hoffman 10\_631358 NO 8201484 NO 1982-1484 19820505 <--NO 152451 NO 152451 FI 8201745 FI 1982-1745 19820518 <--FI 70594 FI 70594 SE 8300288 SE 1983-288 19830120 <--SE 453400 SE 453400 19840130 <--19840130 <--CH 646978 CH 1984-424 CH 1984-425 CH 646979 CH 646980 CH 1984-426 19840130 <--A 19760727 A 19761011 GB 1976-31339 GB 1976-42222 PRIORITY APPLN. INFO.: GB 1977-25700 A 19770620 US 1977-819554 A2 19770727 DK 1977-3378 A 19770726 A 19770726 FI 1977-2280 A 19770727 AT 1977-5509 CH 1977-9307 A 19770727 Approx. 60 bactericidal phosphonic acids, R1ONRXP(O)(OH)2 (R = acyl, R1 = AB H, aralkyl, alkyl, acyl; X = alkylene) and their derivs. were prepared Thus, 6.5 g di-Et 3-(N-butylidenamino)propylphosphonate N-oxide, prepared from butyraldehyde oxime and di-Et 3-bromopropylphosphonate, was hydrolyzed to give 0.48 g 3-(N-hydroxyamino)propylphosphonic acid, which (1.51 g) was acylated with PhOCH2COCl to give 3-(N-hydroxy-Nphenoxyacetylamino) propylphosphonic acid. TТ 66508-34-7P RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and hydrolysis of) 66508-34-7 HCAPLUS RNCarbamic acid, [2-[hydroxy(3-phosphonopropyl)amino]-2-oxoethyl]-, CN C-(phenylmethyl) ester (9CI) (CA INDEX NAME) о он || | Ph-CH<sub>2</sub>-O-C-NH-CH<sub>2</sub>-C-N-(CH<sub>2</sub>)<sub>3</sub>-PO<sub>3</sub>H<sub>2</sub> TΤ 66508-57-4P RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of) 66508-57-4 HCAPLUS RN Phosphonic acid, [3-(formylhydroxyamino)propyl]-, compd. with CN 1,2-ethanediamine (2:1) (9CI) (CA INDEX NAME) CM CRN 66508-53-0 CMF C4 H10 N O5 P OH  $OHC-N-(CH_2)_3-PO_3H_2$ 

CM 2

CRN 107-15-3 CMF C2 H8 N2

H2N-CH2-CH2-NH2

1576-39-2 IT

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with dihaloalkanes)

1576-39-2 HCAPLUS RN

Benzenesulfonamide, 4-methyl-N-(phenylmethoxy)- (9CI) (CA INDEX NAME) CN

98-59-9 IT

> RL: RCT (Reactant); RACT (Reactant or reagent) (reaction with methoxybenzyloxyamines)

RN 98-59-9 HCAPLUS

Benzenesulfonyl chloride, 4-methyl- (9CI) (CA INDEX NAME) CN

L59 ANSWER 35 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

1980:116411 HCAPLUS ACCESSION NUMBER:

DOCUMENT NUMBER: 92:116411

TITLE: Antigen derivatives and pharmaceutical preparations

containing them

Baschang, Gerhard; Dietrich, Felix M.; Gisler, Roland; INVENTOR(S):

Hartmann, Albert; Stanek, Jaroslav; Tarcsay, Lajos

Ciba-Geigy A.-G., Switz. PATENT ASSIGNEE(S):

SOURCE: Eur. Pat. Appl., 131 pp.

CODEN: EPXXDW DOCUMENT TYPE: Patent

LANGUAGE: German

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 3833	A2	19790905	EP 1979-100513	19790221 <

EP 3833 A3 .19800206 EP 3833 B1 19830720 EP 3833 B2 19901219	
EP 3833 B2 19901219	
R: BE, CH, DE, FR, GB, IT, LU, NL, SE	
HU 24554 O 19830328 HU 1979-CI1917 19790203 <	-
HU 182011 B 19831228	
FI 7900584 A 19790825 FI 1979-584 19790221 <	-
FI 66878 B 19840831	
FI 66878 C 19841210	
EP 50703 A2 19820505 EP 1981-102907 19790221 <	-
EP 50703 A3 19820602	
EP 50703 B1 19850410 R: BE, CH, DE, FR, GB, IT, LU, NL, SE	
, , , , , , , , , , , , , , , , , , , ,	
CA 1138436 A1 19821228 CA 1979-321992 19790221 < ES 477977 A1 19800116 ES 1979-477977 19790222 <	
IL 56724 Al 19821231 IL 1979-56724 19790222 <	
DK 7900797 A 19790825 DK 1979-797 19790223 <	
DK 161026 B 19910521	_
DK 161026 C 19911028	
NO 7900626 A 19790827 NO 1979-626 19790223 <	_
NO 151201 B 19841119	
NO 151201 C 19850227	
AU 7944546 Al 19790830 AU 1979-44546 19790223 <	_
AU 527549 B2 19830310	
ZA 7900893 A 19800326 ZA 1979-893 19790223 <	_
DD 141616 C 19800514 DD 1979-211204 19790223 <	
AT 7901420 A 19810415 AT 1979-1420 19790223 <	
AT 364718 B 19811110	
SU 1055312 A3 19831115 SU 1979-2739298 19790223 <	_
JP 54141718 A2 19791105 JP 1979-21281 19790224 <	_
JP 01030809 B4 19890622	
PL 123315 B1 19821030 PL 1979-213696 19790224 <	_
GB 2015534 A 19790912 GB 1979-6649 19790226 <	-
JP 55500336 T2 19800612 JP 1979-500753 19790518 <	-
ES 483558 A1 19800416 ES 1979-483558 19790822 <	-
NO 7903993 A 19790827 NO 1979-3993 19791207 <	-
NO 151088 B 19841029	
NO 151088 C 19850206	
DK 8000086 A 19800108 DK 1980-86 19800108 <	
AT 8102297 A 19830515 AT 1981-2297 19810522 <	-
AT 373265 B 19840110	
AT 8102298 A 19830515 AT 1981-2298 19810522 <	-
AT 373266 B 19840110	
AT 8102299 A 19830515 AT 1981-2299 19810522 < AT 373267 B 19840110	-
US 4397844 A 19830809 US 1981-303244 19810917 < CA 1183528 A2 19850305 CA 1982-403054 19820514 <	
US 4446128 A 19840501 US 1982-379404 19820518 <	
US 4574058 A 19860304 US 1983-477281 19830321 <	
PRIORITY APPLN. INFO.: CH 1978-2035 19830321	
CH 1978-3777 19780407	
CH 1978-5394 19780518	
CA 1979-321992 A3 19790221	
EP 1979-100513 A 19790221	
US 1979-14190 A3 19790222	
AT 1979-1420 A 19790223	
WO 1979-CH71 W 19790518	
US 1981-303244 A 19810917	
AB Antigen conjugates of muramylpeptides were prepared Thus,	

AB Antigen conjugates of muramylpeptides were prepared Thus, 2-acetamido-3-O-{[L-1-(D-1-carbamoyl-3-carboxypropyl)carbamoylethyl]carbam

oylmethyl $\}$ -2-deoxy-D-glucose [72768-58-2] was treated with N-hydroxysuccinimide and the ester [72781-58-9] treated with bovine serum albumin to give a conjugate containing .apprx.60  $\mu$ g muramylpeptide/mg.

IT 2389-49-3

RN 2389-49-3 HCAPLUS

CN L-Lysine, N6-[(1,1-dimethylethoxy)carbonyl]-N2-[(phenylmethoxy)carbonyl]-,
 methyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 24828-95-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and deblocking of)

RN 24828-95-3 HCAPLUS

CN Carbamic acid, [(1S)-1-(aminocarbonyl)-5-[[(1,1-dimethylethoxy)carbonyl]amino]pentyl]-, phenylmethyl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 72781-52-3P

RN 72781-52-3 HCAPLUS

CN L-Lysinamide, N6-[N2-[N-[N-acetyl-1-0-(phenylmethyl)- $\alpha$ -normuramoyl]-L-alanyl]-D- $\alpha$ -glutaminyl]-N2-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

PAGE 1-A

PAGE 1-B

IT 67917-53-7P

RN 67917-53-7 HCAPLUS

CN Carbamic acid, [5-amino-1-(aminocarbonyl)pentyl]-, phenylmethyl ester, (S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$H_2N$$
 $(CH_2)_4$ 
 $S$ 
 $NH_2$ 
 $HN$ 
 $O$ 
 $Ph$ 

IT 333-18-6 42854-62-6

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with muramylpeptide derivative)

RN 333-18-6 HCAPLUS

CN 1,2-Ethanediamine, dihydrochloride (9CI) (CA INDEX NAME)

 $H_2N-CH_2-CH_2-NH_2$ 

●2 HCl

RN 42854-62-6 HCAPLUS

CN L-Alanine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 17831-01-5 CMF C10 H13 N O2

Absolute stereochemistry. Rotation (-).

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L59 ANSWER 36 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1980:94659 HCAPLUS

DOCUMENT NUMBER: 92:94659

TITLE: Building units for oligosaccharides, XVIII. Synthesis

of 4-0-amino acid esters and 4-0-urethanes of garamine

AUTHOR(S): Paulsen, Hans; Boettcher, Henning

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Univ. Hamburg, Hamburg,

D-2000/13, Fed. Rep. Ger.

SOURCE: Chemische Berichte (1979), 112(12), 3864-78

CODEN: CHBEAM; ISSN: 0009-2940

DOCUMENT TYPE: Journal LANGUAGE: German

GI

The garamine I was obtained by CF3CO2H hydrolysis of 2',4',5'-tri-O-benzyl-1,2'',3,3',6''-pentakis-N-(benzyloxycarbonyl)gentamycin C. I was converted to esters and urethanes which on hydrogenation gave free 4-O-aminoacyl- and 4-O-carbamoylgaramines.

IT 7444-16-8

RL: RCT (Reactant); RACT (Reactant or reagent)

(esterification of tribenzyltris(benzoyloxycarbonyl)garamine by)

RN 7444-16-8 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]-, anhydride (9CI) (CA INDEX NAME)

IT 72732-82-2P 72732-84-4P 72732-94-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP

(Preparation); RACT (Reactant or reagent)

(preparation and deblocking of)

RN 72732-82-2 HCAPLUS

CN D-ribo-Heptose, 2,3,4,6,7-pentadeoxy-6-[methyl[(phenylmethoxy)carbonyl]ami no]-2-[[(phenylmethoxy)carbonyl]amino]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 72732-84-4 HCAPLUS

CN Glycine, N-[(phenylmethoxy)carbonyl]-, 4-ester with 2-deoxy-6-0-[3-deoxy-4-C-methyl-3-[methyl[(phenylmethoxy)carbonyl]amino]-2,4-bis-0-(phenylmethyl)-β-L-arabinopyranosyl]-N,N'-bis[(phenylmethoxy)carbonyl]-5-0-(phenylmethyl)-D-streptamine (9CI) (CA INDEX NAME)

RN 72732-94-6 HCAPLUS

CN D-Streptamine, 2-deoxy-6-O-[3-deoxy-4-C-methyl-3 [methyl[(phenylmethoxy)carbonyl]amino]-2,4-bis-O-(phenylmethyl)-β-L arabinopyranosyl]-N,N'-bis[(phenylmethoxy)carbonyl]-5-O-(phenylmethyl)-,
 4-[[6-oxo-6-(phenylmethoxy)-5-[[(phenylmethoxy)carbonyl]amino]hexyl]carbam
 ate], (S)- (9CI) (CA INDEX NAME)

IT 23571-07-5

RL: RCT (Reactant); RACT (Reactant or reagent) (reaction of, with imidazoleylcarbonylgaramine derivs.)

RN 23571-07-5 HCAPLUS

CN 1,2-Ethanediamine, bis(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 107-15-3 CMF C2 H8 N2

H2N-CH2-CH2-NH2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

IT 1738-76-7 5361-91-1 16964-83-3 26727-22-0

RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction of, with imidazolylcarbonylgaramine derivs.)

RN 1738-76-7 HCAPLUS

CN Glycine, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME) CM 1

CRN 1738-68-7 CMF C9 H11 N O2

$$\begin{array}{c} \text{O} \\ \| \\ \text{Ph-CH}_2\text{-O-C-CH}_2\text{-NH}_2 \end{array}$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 5361-91-1 HCAPLUS

CN L-Lysine, N2-[(phenylmethoxy)carbonyl]-, phenylmethyl ester, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 5591-94-6 CMF C21 H26 N2 O4

Absolute stereochemistry. Rotation (-).

$$H_2N$$
 $(CH_2)_4$ 
 $S$ 
 $O$ 
 $Ph$ 
 $O$ 
 $Ph$ 

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 16964-83-3 HCAPLUS

CN L-Lysine, N6-[(phenylmethoxy)carbonyl]-, phenylmethyl ester, mono(4-methylbenzenesulfonate) (9CI) (CA INDEX NAME)

CM 1

CRN 24458-14-8 CMF C21 H26 N2 O4

Absolute stereochemistry.

$$\begin{array}{c|c} & & & & \\ & & & \\ \text{Ph} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

RN 26727-22-0 HCAPLUS

CN Butanoic acid, 4-amino-, phenylmethyl ester, 4-methylbenzenesulfonate (9CI) (CA INDEX NAME)

CM 1

CRN 46347-99-3 CMF C11 H15 N O2

CM 2

CRN 104-15-4 CMF C7 H8 O3 S

L59 ANSWER 37 OF 37 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1977:121758 HCAPLUS

DOCUMENT NUMBER: 86:121758

TITLE: Amino acids and peptides. CXXXV. Synthesis of

derivatives and peptides of  $\alpha$ -amino- $\beta$ -guanidinopropionic acid and  $\alpha$ -amino- $\gamma$ -

guanidinobutyric acid

AUTHOR(S): Brtnik, F.; Zaoral, M.

CORPORATE SOURCE: Inst. Org. Chem. Biochem., Czech. Acad. Sci., Prague,

Czech.

SOURCE: Collection of Czechoslovak Chemical Communications (

**1976**), 41(10), 2969-77

CODEN: CCCCAK; ISSN: 0010-0765

DOCUMENT TYPE: Journal LANGUAGE: English

AB The reaction of H2NCH2CH2CN (NHCO2Ch2Ph) CO2H with MeOC (NH2):NNO2 in aqueous

NaOH gave H2NC(:NNO2)NHCH2CH(NHCO2CH2Ph)CO2H which was condensed with H-Gly-NH2 to give a dipeptide which was deblocked with HBr/AcOH and

condensed with Z-Pro-OH (Z = PhCH2O2C) to give Z-Pro-

NHCH[CH2NHC(:NNO2)NH2]CO-Gly-NH2. H-Pro-D-NHCH[CH2NHC(:NNO2)NH2]CO-Gly-NH2 was prepared analogously from D-H2NCH2CH(NHZ)CO2H and converted to PhCH2SCH2CH2CO-Tyr-Phe-Glu-Asn-Cys(CH2Ph)-Pro-D-NHCH[CH2NHC(:NNO2)NH2]CO-

Gly-NH2.

IT 55264-42-1

RL: RCT (Reactant); RACT (Reactant or reagent)

(peptide coupling of)

RN 55264-42-1 HCAPLUS

CN Acetamide, 2-amino-, monohydrobromide (9CI) (CA INDEX NAME)

## HBr

IT 13558-07-1P 16947-86-7P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and detosylation of)

RN 13558-07-1 HCAPLUS

CN Butanoic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-[[(4methylphenyl)sulfonyl]amino]-, (S)- (9CI) (CA INDEX NAME)

RN 16947-86-7 HCAPLUS

CN L-Alanine, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 49855-91-6P 62234-42-8P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation and partial deblocking of)

RN 49855-91-6 HCAPLUS

CN Butanoic acid, 4-[[(1,1-dimethylethoxy)carbonyl]amino]-2-[[(phenylmethoxy)carbonyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 62234-42-8 HCAPLUS

CN Glycinamide, 3-[[imino(nitroamino)methyl]amino]-N[(phenylmethoxy)carbonyl]-D-alanyl- (9CI) (CA INDEX NAME)

$$H_{2}N$$
 $H_{1}$ 
 $H_{2}N$ 
 $H_{3}$ 
 $H_{4}$ 
 $H_{5}$ 
 $H_$ 

Absolute stereochemistry.

RN 62234-38-2 HCAPLUS

CN L-Alanine, 3-[[imino(nitroamino)methyl]amino]-N-[(phenylmethoxy)carbonyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ O_2N & & & \\ & & & \\ NH & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & &$$

RN 62234-39-3 HCAPLUS

CN D-Alanine, 3-[[imino(nitroamino)methyl]amino]-N-[(phenylmethoxy)carbonyl]-(9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 62234-40-6P

RN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation and reaction with nitroisourea) 62234-40-6 HCAPLUS

CN Butanoic acid, 4-amino-2-[[(phenylmethoxy)carbonyl]amino]-, (2S)- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

IT 35761-26-3P 62234-37-1P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with nitroisourea derivative)

RN 35761-26-3 HCAPLUS

CN L-Alanine, 3-amino-N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).

RN 62234-37-1 HCAPLUS

CN D-Alanine, 3-amino-N-[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

IT 16947-84-5P 62234-36-0P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction with trifluoroacetic acid)

RN 16947-84-5 HCAPLUS

CN L-Alanine, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-N[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

RN 62234-36-0 HCAPLUS

CN D-Alanine, 3-[[(1,1-dimethylethoxy)carbonyl]amino]-N[(phenylmethoxy)carbonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

IT 62234-31-5P 62234-41-7P 62234-44-0P

RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of)

RN 62234-31-5 HCAPLUS

CN Butanoic acid, 4-[[imino(nitroamino)methyl]amino]-2-[[(phenylmethoxy)carbonyl]amino]-, (S)-, compd. with Ncyclohexylcyclohexanamine (1:1) (9CI) (CA INDEX NAME)

CM 1

CRN 62234-30-4 CMF C13 H17 N5 O6

Absolute stereochemistry.

CM 2

CRN 101-83-7 CMF C12 H23 N

RN 62234-41-7 HCAPLUS

CN Glycinamide, 3-[[imino(nitroamino)methyl]amino]-N[(phenylmethoxy)carbonyl]-L-alanyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

RN 62234-44-0 HCAPLUS

CN Glycinamide, N4-[imino(nitroamino)methyl]-N2-[(phenylmethoxy)carbonyl]-L-2,4-diaminobutanoyl- (9CI) (CA INDEX NAME)

Absolute stereochemistry.

$$\begin{array}{c|c} & & & \\ &$$

IT 21753-19-5

RL: RCT (Reactant); RACT (Reactant or reagent)
 (reaction of, with tert-butoxycarbonyl azide)

RN 21753-19-5 HCAPLUS

CN L-Alanine, 3-amino-N-[(4-methylphenyl)sulfonyl]- (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (-).